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Towards Dynamic Dimension Reduction in Reactive Flow Problems

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Abstract

The paper addresses the possibilities of reducing the overall number of degrees of freedom in large scale reactive flow computations. Attention focusses on the dimension reduction technique ILDM due to MAAS AND POPE, which treats certain automatically detected fast dynamic components as algebraic equations (so-called slow manifold). In earlier papers, the dimension of the reduction had been kept constant throughout each computation. Recently, a mathematically sound and nevertheless cheap dimension monitor for the chemistry part only has been suggested by DEUFLHARD AND HEROTH. The present paper reports about first steps taken towards the implementation of that monitor into a flame code. Moreover, a sparse grid storage scheme is advocated and analyzed in view of the construction of efficient table look-ups for nested manifolds.

1 Introduction

The reduction of chemical reaction models is a hard challenging task in the simulation of complex reaction kinetics. This is due to the fact that the simulation of multi-dimensional reacting flows involving several hundreds of chemical species (e.g. in combustion processes) with detailed models for the chemical processes will remain impossible in the near future. One standard mathematical tool for the reduction of chemical reaction models is the well-known technique of *quasi-steady-state approximation* (QSSA), which produces a differential-algebraic system

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(DAE). It is typically based on chemical insight into the reaction mechanism. Unfortunately, chemical insight often does not assure that the thus obtained DAE has a *unique* solution (index 1 problem) – compare e.g. the illustrating example in [6]. Moreover, even when the index is 1, there can be a quite large difference between the solutions of the ODE and the associated DAE obtained from the QSSA procedure – which led FARROW AND EDELSON [9] to talk about "QSSA – fact or fiction".

Difficulties of this kind are avoided by the recent method of *intrinsic low-dimensional manifolds* (ILDm) as suggested in [13]. This method uses an *automatic formal splitting*: a real Schur decomposition of the Jacobian is performed to identify the *slow* and *fast* components. The manifold defined by the algebraic conditions for the fast components can be tabulated for further use in the computation of reacting flows. After projection of the partial differential equation onto the manifold, one is left with solving a system for the parameters only [14]. The state of the chemical part of the system can then be computed from the parameters by a mere *table look-up*.

In [7], the involved automatic splitting has been analyzed carefully: the mathematically sound and computationally cheap splitting monitor derived there is briefly revisited below in Section 2. The results there apply to the spatially homogenous case (pure ODE/DAE case). The present paper reports about first steps taken in the direction of the true PDE case, wherein the question of algorithmic realization of the necessary table look-up is crucial (Section 3). As reported in [15], $d = 6$ or even more parameters may be needed in the slow part of the system. Therefore the task is to set up and store a table with up to 6 parameters and up to 1000 reals per interpolation point. If one chooses a regular grid with meshsize h (in the space of the parameters) for interpolation, the number of knots in the grid grows like h^{-d} and soon exceeds any reasonable memory resources. A first way out of this undesirable limitation has been suggested in [15]. There the parameter domain is split into quite few coarse cells and higher order interpolation polynomials are used. The thus obtained savings are due to the fact that larger meshsizes can be taken to meet a prescribed accuracy requirement. However, in this approach the number of knots is still determined by h^{-d} in each cell. A more promising approach to be advocated herein is to solve this interpolation problem by means of so-called *sparse grids* – see ZENGER [17]. Such grids can be incorporated into any given coarse cell and combined with higher order polynomials as well. Their striking advantage is that the number of knots in a sparse grid only grows like $h^{-1}(\log_2 h^{-1})^{d-1}$, which means that the curse of dimension can be overcome. Details of first considerations in this direction are given in Section 3.

2 Splitting Monitor

In this section we briefly revisit the main results of [7]. Consider the following initial value problem (IVP) for ordinary differential equations (ODEs)

$$\dot{x} = F(x), \quad x(0) = x^0 \quad (1)$$

wherein $x \in \mathbf{R}^n$ may represent concentrations of chemical species, temperature, pressure etc. When the system is stiff, it will have so-called "fast" components expected to reach their steady state after a short transient period.

Automatic splitting algorithm. In [12], fast and slow components are split by application of a *real block-Schur decomposition*: starting from the matrix $A = F_x(x^0)$, this decomposition supplies certain nonsingular matrices T_d , which generate the following block splitting:

$$T_d^{-1} A T_d = S = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{22} \end{pmatrix}$$

The splitting dimension d is just the dimension of the submatrix S_{11} . The eigenvalues λ can be grouped according to their real parts such that some splitting parameter μ can be defined as

$$\mu := \max_{\lambda \in S_{22}} \Re \lambda < 0 \quad \text{and} \quad \min_{\lambda \in S_{11}} \Re \lambda > \mu.$$

This block decomposition is performed in *two* steps: First a real Schur decomposition yields

$$Q_d^T A Q_d = \bar{S} = \begin{pmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{pmatrix}$$

with an orthogonal matrix Q_d ; in a second step the desired block structure is obtained by solving the Sylvester equation

$$S_{11}Z - ZS_{22} = -S_{12}$$

and setting

$$T_d^{-1} = \left(I - \begin{pmatrix} 0 & Z \\ 0 & 0 \end{pmatrix} \right) Q_d^T \quad \text{and} \quad T_d = Q \left(I + \begin{pmatrix} 0 & Z \\ 0 & 0 \end{pmatrix} \right).$$

The condition number of T_d , which depends on Z only, is a means to check for the "spectral gap condition" known from mathematical analysis. In this way, new coordinates

$$\begin{pmatrix} y \\ z \end{pmatrix} := T_d^{-1} x, \quad (2)$$

arise naturally together with the perturbation parameter

$$\varepsilon := 1/\mu$$

and lead to the canonical form

$$\begin{aligned} \dot{y} &= f(y, z), \\ \varepsilon \dot{z} &= g(y, z), \quad (y, z)(0) = T_d^{-1}x^0, \end{aligned} \tag{3}$$

The QSSA assumption now yields the associated DAE

$$\begin{aligned} \dot{y}_0 &= f(y_0, z_0), & y_0(0) &= \bar{y}^0 \\ 0 &= g(y_0, z_0), & z_0(0) &= \bar{z}^0, \end{aligned} \tag{4}$$

where the initial values (\bar{y}_0, \bar{z}_0) are assumed to be consistent, i.e.

$$(\bar{y}_0, \bar{z}_0) \in \mathcal{M}_d := \{(y, z) : g(y, z) = 0\}.$$

Now, d can always be chosen such that g_z is *regular* in some neighborhood of the initial value, which means that this system has index 1 and therefore a locally unique solution.

Estimation of the QSSA Error. Structurally, the usual sequence of integration steps

$$\text{IVP}_1 \longrightarrow \text{IVP}_2 \longrightarrow \dots \longrightarrow \text{IVP}_N \longrightarrow \text{solution}$$

is replaced here by a sequence of the kind

$$\begin{array}{ccccccc} \text{IVP}_1 & & \text{IVP}_2 & & \dots & & \text{IVP}_N & & \text{solution} \\ \downarrow \nearrow & & \downarrow \nearrow & & \dots & & \downarrow \nearrow & & \\ \text{DAE}_1 & & \text{DAE}_2 & & \dots & & \text{DAE}_N & & \end{array}$$

wherein a projection of the new initial values onto the new algebraic manifolds will be necessary at each integration step. Clearly, the approximation errors play a similar role as local discretization errors. Numerical integrators control *local discretization error estimates* ε_k by testing $\varepsilon_k \leq \text{TOL}$ with TOL being a user prescribed error tolerance. In our situation, the local errors *additionally* contain errors introduced by the switching from an ODE system of type (3) to a DAE system of type (4). These errors need to be estimated in a cheap and reliable way in order to enable a theoretically backed splitting into slow and fast components of the dynamical system.

Let (y, z) denote the solution of the ODE system (3) and (y_0, z_0) the solution of the DAE system (4) and let τ be the timestep chosen by the applied numerical

integrator. Then the QSSA error of interest after one integration step is required to satisfy

$$\alpha = \|(y, z)(\tau) - (y_0, z_0)(\tau)\| \leq \text{TOL}.$$

In order to estimate α we apply standard results from singular perturbation theory, in particular a quite well-known result of VASIL'eva [16]. If we assume the right-hand side F to be at least twice differentiable, the following asymptotic expansion is known to hold:

$$\begin{aligned} y(t) &= y_0(t) + \varepsilon(y_1(t) + \eta_1(t/\varepsilon)) + O(\varepsilon^2) \\ z(t) &= z_0(t) + \zeta_0(t/\varepsilon) + \varepsilon(z_1(t) + \zeta_1(t/\varepsilon)) + O(\varepsilon^2) \end{aligned}$$

Here ζ_0 , ζ_1 and η_1 are exponentially decaying terms in the sense that with $s = t/\varepsilon$ we have

$$\|\zeta_0(s)\| \leq \|\zeta_0(0)\| e^{-\kappa s}, \quad \|\eta_1(s)\| \leq \|\eta_1(0)\| e^{-\kappa s} \quad (5)$$

with $\kappa \approx 1$ due to the scaling of ε . We assume $\kappa = 1$ and focus on the approximation error in the slow components. Furthermore, the analysis is restricted to the first order error term $y_1(\tau)$. Thus we arrive at the estimate

$$\alpha \doteq \varepsilon \|y_1(\tau)\|.$$

VASIL'eva's theorem shows that y_1 is the solution of a linear IVP driven by the slow components. Any useful stepsize selection device will keep the error amplification of that problem approximately at 1, so that we finally arrive at the next estimate

$$\alpha \approx \varepsilon \|y_1(0)\|.$$

In order to compute this estimate, some calculations are necessary, for details see [7]. We end up with

$$y_1(0) \approx \Delta f := (f(y(0), z(0)) - f(y(0), z_0(0))),$$

which implies the cheaply available estimate

$$[\alpha] = \varepsilon \|\Delta f\| \leq \text{TOL}. \quad (6)$$

If this condition is violated, the splitting should be performed again and the dimension d should be *possibly increased*. Note, however, that this singular perturbation treatment is only valid for the pure ODE/DAE case. Its generalization to the degenerate PDE case is non-trivial.

Numerical Experiments. The dynamic dimension reduction algorithm has been implemented within the linearly implicit Euler discretization with two extrapolation steps only, thus restricting the discretization order to $p = 3$. For the user prescribed accuracy we always set $\text{TOL} = 10^{-2}$.

Example 1: Hydrogen-Oxygen Combustion [10]. This problem consists of $n = 8$ chemical species (and ODEs) and 37 elementary chemical reactions. The reaction mechanism is part of a system investigated in [13] and [12]. In [10] it is shown that in this example the traditional analytic QSSA fails to be applicable. It is therefore interesting to see the performance of the adaptive tool. In Fig. 1, the numerical solution of the sequence of DAE systems is represented graphically; it agrees perfectly with the results obtained from solving the original ODE system also plotted in the same figure. The small ignition zone in time is nicely resolved by the stepsize control, which demonstrates that our dimension reduction mechanism does not affect the efficiency of the integrator. Only *two* parameters are neces-

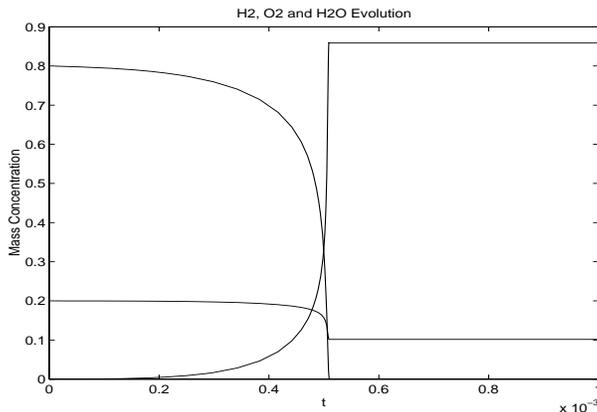


Figure 1: Species concentrations H_2 , O_2 and H_2O

sary in the reduced system to describe this combustion problem. (It should be noted that we treated the invariants of the system independently.) The adaptive method works satisfactorily: once the hydrogen is exhausted, the system reaches its fixed point with $d = 0$. If we force $d = 1$ throughout the whole integration

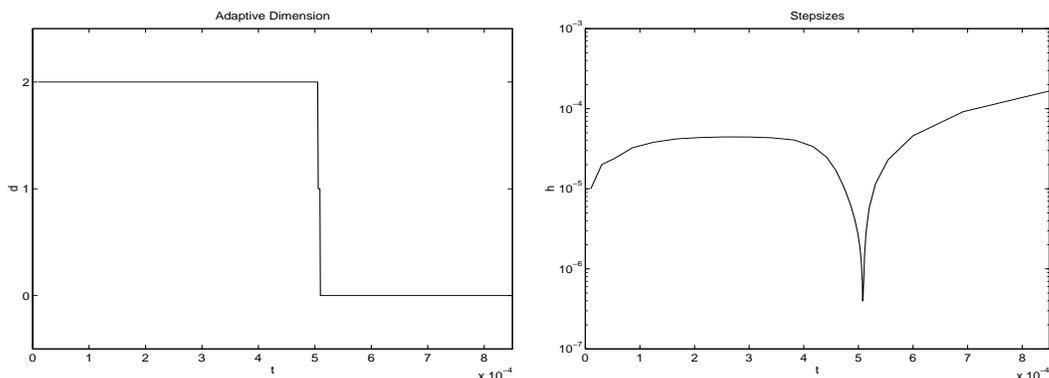


Figure 2: Splitting dimension and timestep behavior for block-Schur decomposition at each discretization step (41 steps)

and turn off the control of the QSSA error we get no result at all, because the

stepsizes shrink below 10^{-20} immediately. Therefore, we conclude that $d = 2$ is a minimum dimension necessary to model this combustion process correctly. The success of the automatic dimension reduction algorithm can also nicely be seen by comparison with the quite sophisticated analytical singular perturbation treatment of HOPPENSTEADT ET AL. in [10].

Example 2: Thermal decomposition of n-hexane (due to ISBARN, EDERER AND EBERT [11]). In this example the automatic reduction method does not lead to a strong reduction of the chemical system. The problem consists of $n = 59$ species and 240 elementary chemical reactions. The temperature was set to 728 K. In order to establish the right hand side of the ODE system correctly the algorithm was implemented within the software package LARKIN [4, 2]. Again the numerical results obtained by the dynamic dimension reduction method were indistinguishable from those obtained by solving the original ODE system. The associated dynamic dimension sequence is plotted in Fig. 3 for two different time intervals. In this example, the slow components of the system were integrated numerically by an explicit Euler scheme. There is no strong reduction in the

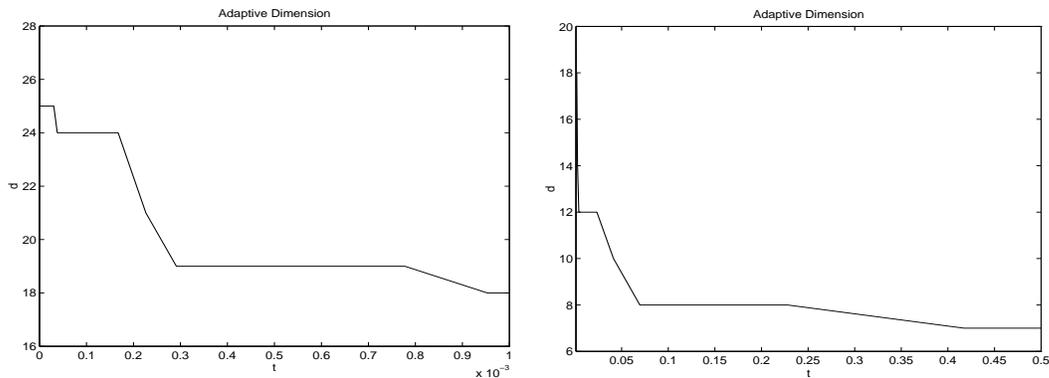


Figure 3: Dynamic dimension reduction over two time intervals.

initial phase. This is due to the fact that here more than 15 eigenvalues are so close to 0 that the corresponding transformed components may be regarded as being "nearly conserved quantities". Methods, which allow to decouple such slow processes, can be designed and would lead to a further dimension reduction.

In the above problems, the algebraic equations defining the manifold have been treated by application of a Newton-like method in the course of the numerical integration. This would be too expensive in PDE calculations, as already mentioned in the Introduction. Rather, in this case, a considerable computational speed-up can be achieved by parametrizing the manifold in advance – so that during the numerical PDE integration only table look-ups are necessary to take care of the algebraic parts. Proceeding like that also nicely reflects the fact that the chemical part is a point operation within the PDE - in contrast to the physical part, which reflects the spatial spread of the problems. The question left to discuss is then

how to store the parametrized manifold in such a way that it can be efficiently evaluated within the PDE computation for variable dimension. This question is addressed in the next section.

3 Sparse Grid Storage Scheme

Sparse grids were introduced by ZENGER in [17] to reduce the amount of knots needed in finite element calculations. Starting with a hierarchal basis decomposition of the considered finite element space one can compare the contributions of the subspaces. It turns out that large savings are possible if the subspaces are grouped in a certain way.

To see how this works, let u be a sufficiently smooth function on $[0, 1]^2$ vanishing on the boundary of the cube. In order to interpolate to u we introduce a grid $G_{n,m}$ with meshsizes $h_1 = 2^{-n}$ and $h_2 = 2^{-m}$ on $[0, 1]^2$. Suppose that we seek for an interpolating function u_n in the space of piecewise bilinear functions $S_{n,m}$ associated with the grid. To achieve the so-called *hierarchal basis decomposition* of $S_{n,m}$, let $T_{i,j}$ denote the subspace of $S_{n,m}$ that vanishes on the subgrids $G_{n-1,m}$ and $G_{n,m-1}$. In Fig. 4, the subspaces $T_{i,j}$ are arranged in a matrix scheme to give an idea of that decomposition.

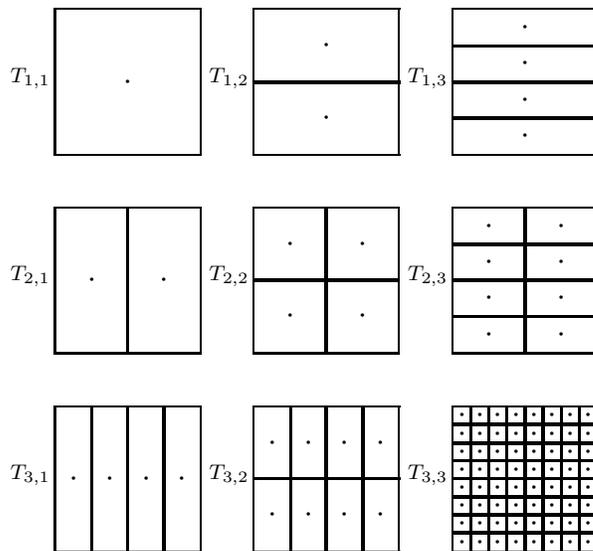


Figure 4: Decomposition of $S_{3,3}$ into subspaces $T_{i,j}$.

Herein each rectangle denotes the support of a basis function $b \in T_{i,j}$. Each basis

function $b \in T_{i,j}$ is bilinear, has the value one in the midpoint of the rectangle (indicated by a dot) and the value zero in the vertices. With the choice $m = n$ these subspaces decompose $S_{n,n}$ into a direct sum:

$$S_{n,n} = \sum_{i=1}^n \sum_{j=1}^n T_{i,j}.$$

The interpolant u_n to u is decomposed analogously

$$u_n = \sum_{i=1}^n \sum_{j=1}^n u_{i,j} \quad u_{i,j} \in T_{i,j}.$$

It is shown in [17] that the subspaces $T_{i,j}$ differ considerably in their contribution $\|u_{i,j}\|_\infty = O(4^{-i-j-1})$ to u_n . Therefore in Fig. 4, the approximation may be improved without increasing the number of knots by dropping the space $T_{3,3}$ which has a contribution of order 4^{-7} and adding the spaces $T_{4,1}$ and $T_{1,4}$, having a contribution of order 4^{-6} each. Generally speaking, one keeps the upper left triangle of the matrix scheme including the diagonal and drops the spaces in the lower right triangle:

$$\tilde{S}_n := \sum_{i+j \leq n+1} T_{i,j}.$$

The sparse grids are the grids associated with \tilde{S}_n . They consist of much less points than the full grid $G_{n,n}$ associated with the Space $S_{n,n}$. As an example, Fig. 5 shows the sparse grid for \tilde{S}_4 .

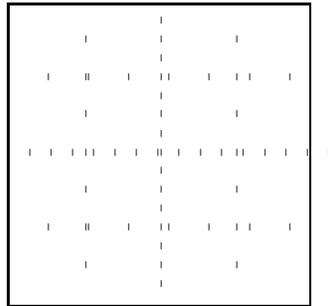


Figure 5: Sparse grid for \tilde{S}_4 .

Properties. In [3], BUNGARTZ analyzes sparse grids for arbitrary dimensions d , defined by

$$\tilde{S}_n := \sum_{i_1 + \dots + i_d \leq n+d-1} T_{i_1, \dots, i_d}.$$

The striking property is that the number of grid points $N(d)$ increases rather slowly with d , whereas the order of approximation is only diminished by a logarithmic

factor. Instead of the usual number $N(d) = O(h^{-d})$ of knots for full grids, we only have

$$N(d) = O(h^{-1}(\log_2 h^{-1})^{d-1})$$

in the case of sparse grids. This is also correct if we drop the condition that u should vanish on the boundary. Nevertheless, if u is sufficiently smooth, the approximation order of the sparse grid approach is

$$\|u - \tilde{u}_n\|_\infty = O(h^2(\log_2 h^{-1})^{d-1}).$$

which is almost as good as the order $O(h^2)$ for the full grid. Sufficiently smooth means that the mixed derivative $\frac{\partial^{2d}u}{\partial^2x_1 \dots \partial^2x_d}$ remains bounded. In Fig. 6, we list the number of knots in the interior of the cube for different dimensions and meshsizes $h = 2^{-n}$.

$n \setminus d$	1	2	3	4	5	6
1	1	1	1	1	1	1
2	3	5	7	9	11	13
3	7	17	31	49	71	97
4	15	49	111	209	351	545
5	31	129	351	769	1471	2561
6	63	321	1023	2561	5503	10625
7	127	769	2815	7937	18943	40193
8	255	1793	7428	23297	61183	141569
9	511	4097	18943	65537	187903	471041
10	1023	9217	47103	178177	553983	1496065

Figure 6: Inner grid points for several dimensions with $h = 2^{-n}$

In dimension 6 with meshsize $h = 2^{-6}$ e.g., we need 10625 knots in the interior of the six-dimensional cube instead of $(2^6 - 1)^6 \approx 6 \cdot 10^{10}$ knots in the full grid with the same meshsize. For such large meshsizes however, the approximation order is diminished drastically by the logarithmic part. But, as already developed in [3], one can increase the order to $O(h^3(\log_2 h^{-1})^{d-1})$ or $O(h^4(\log_2 h^{-1})^{d-1})$ respectively using quadratic or cubic basis functions. Additionally, an adaptive strategy can be designed to skip all knots or subspaces, wherein the contributions $u_{i,j}$ become small. Moreover, local extrapolation techniques as introduced by BABUSKA AND RHEINBOLDT [1] can be used to increase *local* orders.

The above sparse grid technique works well in tensorproduct spaces. For this reason, we hope to extend it in such a way that a recursive table look-up for *nested* manifolds is possible.

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