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ERROR ESTIMATION FOR REDUCED ORDER MODELS OF DYNAMICAL SYSTEMS *

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Abstract. The use of reduced order models to describe a dynamical system is pervasive in science and engineering. Often these models are used without an estimate of their error or range of validity. In this paper we consider dynamical systems and reduced models built using proper orthogonal decomposition. We show how to compute estimates and bounds for these errors, by a combination of small sample statistical condition estimation and error estimation using the adjoint method. Most importantly, the proposed approach allows the assessment of *regions of validity* for reduced models, i.e., ranges of perturbations in the original system over which the reduced model is still appropriate. Numerical examples validate our approach: the error norm estimates approximate well the forward error while the derived bounds are within an order of magnitude.

Key words. model reduction, proper orthogonal decomposition, small sample statistical condition estimation, adjoint method

AMS subject classifications. 65L10, 65L99

1. Introduction.

Model reduction of dynamical systems described by differential equations is ubiquitous in science and engineering [1]. Reduced models are used for efficient simulation [12, 24] and control [13, 22]. Moreover, the process of creating low-order models forces the researcher to isolate and quantify the dominant physical mechanisms, revealing effective design decisions that would not have been identified through numerical simulation, experiments or "black box" optimization methods [23].

The Proper Orthogonal Decomposition (POD) method has been used extensively in a variety of fields including fluid dynamics [18], identification of coherent structures [8, 16], control [21] and inverse problems [14]. The method has been employed for industrial applications such as supersonic jet modeling [4], turbine flows [5], thermal processing of foods [2], and study of the dynamic wind pressures acting on buildings [11], to name only a few. A detailed description [8] of the POD approach as a reduction method shows that, for a given number of modes, POD is the most efficient choice among all linear decompositions in the sense that it retains, on average, the greatest possible kinetic energy.

As soon as one contemplates the use of a reduced model, questions concerning the quality of the approximation become paramount. To judge the quality of the reduced model, it is important to estimate its error. An algorithm for estimating the error of a class of reduction methods based on projection techniques was presented in [25]. In this approach, the original problem is linearized around the initial time. The resulting first-order error estimates are valid for only a small number of time steps (during which the Jacobian matrix can be considered constant). First-order estimates

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of POD errors were used in [15] to extend the concept of domain decomposition as a dynamic, *a posteriori* verification and, if necessary, correction of the approximate solution. Error estimates for reduced models, more precisely the error for certain functionals of the solution, were obtained in [19]. The authors employed the dual-weighted-residual method, which makes use of the solution of an adjoint system.

In the context of fluid dynamics, bounds for the errors resulting from POD model reduction of 2-D Navier-Stokes equations were computed in [14]. In that work, the approximation error was decomposed into a contribution that arises due to the POD spatial approximation (measured in terms of the spectral properties specifying the POD basis) and the approximation error due to the backward Euler scheme for time integration. The resulting estimates made use of certain inequalities that, although valid for the nonlinear evolution problem considered, may not be satisfied for other examples. For models that contain discontinuities, for example if the solution involves shocks, it was found in [17] that the POD reduced model was able to represent a shock in a given location only if one of the snapshots used to build the model has a discontinuity in the same location. This may require an unacceptably large number of snapshots to achieve sufficient accuracy of the approximate solution. To overcome this limitation a domain decomposition technique was introduced, using a reduced order model over the majority of the computational domain while solving the full equations in a small region. Given an approximate solution (with unknown accuracy) generated with a set of POD basis functions, the error is estimated by augmenting the POD basis with top hat basis functions and computing the first order change in the solution due to the additional basis functions. By comparing against the results from a solution of known accuracy, such as one of the snapshots used to generate the POD basis, the need for domain decomposition and its spatial extent can be determined.

Bounds of POD errors, but not estimates, were considered in [20], as well as effects (on the reduced order model) of small perturbations in the ensemble of data from which the POD reduced order model was constructed.

In the present work we take the analysis of reduced models one step further by analyzing the influence of perturbations to the original system on the quality of the approximation given by the reduced model. This question is of particular interest in applications (such as control and inverse problems) in which reduced models are used not just to approximate the solution of the original system that provided the data used in constructing the reduced model, but rather to approximate the solution of systems perturbed from the original one. To the best of our knowledge, there are no published results to address the estimation of the model reduction error of such perturbed systems.

We base our approach on a combination of the small sample statistical condition estimation (SCE) method [10] and error estimation using the adjoint method. Using this framework, we define *regions of validity* of the reduced models, that is, ranges of perturbations in the original system over which the reduced model is still appropriate. We consider perturbations in both the initial conditions and in parameters describing the dynamical system itself. The proposed approach is particularly attractive because the resulting error bounds do not rely on the solution of the perturbed system. In this sense, we provide an *a-priori* assessment of the validity of the model-reduction approximation. We note that our approach is based on linearization. For large enough perturbations, knowledge of the solution of the perturbed system would be required.

Unlike the method presented in [25], our estimates and bounds are valid over the entire time interval considered and not only in a neighborhood of the initial time.

Moreover, we obtain estimates for the continuous error, as opposed to its discrete approximation. Although we study only a particular projection-based model reduction technique (POD) among those considered in [25], the methodology developed here for POD can be easily extended to other types of projection. Compared to the approach taken in [14], our method is applicable to a larger class of problems, our main requirement being that the norm of the POD-based error is small enough for the linearized error equation to be a good enough approximation. Furthermore, our estimates are independent of the time integration method. We note also that our use of adjoint models for error estimation is similar to that employed in [19]. However, as will be seen below, the use of the SCE method enables the derivation of error "condition numbers" and allows effective treatment of the *region of validity* problem.

In the context of integration of ordinary differential equations (ODE), the SCE method combined with the adjoint approach has been used in [3] for estimation and control of the global integration error.

The remainder of this paper is organized as follows. In §2 and §3 we briefly describe the use of POD for model reduction and, respectively, the SCE method for norm estimation. In §3.1 we motivate our proposed approach of using SCE, combined with error estimation using the adjoint method, to estimate the errors due to the use of a reduced order model. In §4 we analyze errors arising purely from the model reduction itself: the total approximation error and the subspace integration error. In §5 we analyze regions of validity of POD reduced models. In §6 we present numerical results for two example problems. The first one is obtained from the semi-discretization of time-dependent partial differential equation (PDE), namely advection-diffusion, while the second example models a pollution chemical reaction mechanism. Finally, §7 summarizes our results and indicates plans of future research.

2. POD-based reduced models. POD provides a method for finding the best approximating affine subspace to a given set of data. When using POD for model reduction of dynamical systems, the data are time snapshots of the solution obtained via numerical simulations or from experiments. Consider the ODE system

$$\frac{dy}{dt} = f(y,t)\,, \quad y(t_0) = y_0\,, \tag{2.1}$$

for $t \in [t_0, t_f]$, with $y, y_0 \in R^n$ and $f : R^n \times R \to R^n$. Consider next the solutions of (2.1) at m time points, collected in the $n \times m$ matrix $\mathcal{Y} = [y(t_1) - \bar{y}, y(t_2) - \bar{y}, \dots y(t_m) - \bar{y}]$, where $\bar{y}$ is the mean of these observations. POD seeks a subspace $S \in R^n$ and the corresponding projection matrix P_S so that the total square distance

$$\|\mathcal{Y} - P\mathcal{Y}\|^2 = \sum_{i=1}^{m} \|\,(y(t_i) - \bar{y}) - P\,(y(t_i) - \bar{y})\,\|^2$$

is minimized. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m \geq 0$ be the ordered eigenvalues of the *correlation matrix* $R = \mathcal{Y}\mathcal{Y}^T$. Then the minimum value of $\|\mathcal{Y} - P\mathcal{Y}\|^2$ over all k-dimensional subspaces S, with $k \leq n$, is given by $\sum_{j=k+1}^{n} \lambda_j$. Moreover, the minimizing S is the invariant subspace corresponding to the eigenvalues $\lambda_1, \dots, \lambda_k$. Using the singular value decomposition (SVD) [6] of the observation matrix, $U^T \mathcal{Y} V = \Sigma$, the projection matrix corresponding to the optimal POD subspace S is obtained as

$$P = \rho\rho^T \in R^{n\times n}\ , \tag{2.2}$$

where ρ is the matrix of projection onto S, the subspace spanned by the reduced basis obtained from the SVD. The matrix $\rho \in R^{n\times k}$ consists of the columns V_i $(i = 1\dots k)$, the singular vectors corresponding to the k largest singular values.

In a coordinate system embedded in S, the projection of a point y onto S is represented by $y^S = \rho^T(y - \bar{y}) \in R^k$, while in the full space, the same projection is expressed as $\tilde{y} = P(y - \bar{y}) + \bar{y} \equiv \rho y^S + \bar{y} \in R^n$.

A POD-based reduced model that approximates the original problem (2.1) can then be constructed [20] by projecting onto S the vector field $f(s, t)$ at each point $s \in S$. If y^S are the subspace coordinates of s, then

$$\frac{dy^S}{dt} = \rho^T f(\rho y^S + \bar{y}, t)\,, \quad y^S(t_0) = \rho^T(y_0 - \bar{y})\,. \tag{2.3}$$

The approximate solution $\hat{y}$ is the solution of the ODE initial-value problem (IVP)

$$\frac{d\hat{y}}{dt} = Pf(\hat{y}, t)\,, \quad \hat{y}(t_0) = P(y_0 - \bar{y}) + \bar{y}\,. \tag{2.4}$$

3. Small sample statistical method for condition estimation. The small sample statistical condition estimation (SCE) method, originally proposed in [10], offers an efficient means for condition estimation for general matrix functions, at the cost of allowing moderate relative errors in the estimate. The basic idea is described below (for complete details, see [7, 10]).

For any vector $v \in R^n$, if z is selected uniformly and randomly from the unit sphere S_{n-1}, the expected value of $z^T v$ is proportional to the norm of v:

$$E(|z^T v|) = W_n ||v|| \ .$$

The *Wallis factor* W_n is defined as

$$W_1 = 1\,, \quad W_n = \begin{cases} \dfrac{1\cdot 3\cdots(n-2)}{2\cdot 4\cdots(n-1)} & n \text{ odd} \\ \dfrac{2}{\pi}\dfrac{2\cdot 4\cdots(n-1)}{1\cdot 3\cdots(n-2)} & n \text{ even} \end{cases} .$$

We estimate the norm $||v||$ using the expression $\xi = \dfrac{|z^T v|}{W_n}$, with $W_n \approx \sqrt{\dfrac{2}{\pi(n-\frac{1}{2})}}$. This estimate is first order in the sense that the probability of a relative error in the estimate is inversely proportional to the size of the error. That is, for $\gamma > 1$

$$Pr\left(\frac{||v||}{\gamma} \le \xi \le \gamma||v||\right) \ge 1 - \frac{2}{\pi\gamma} + O\left(\frac{1}{\gamma^2}\right) \ .$$

Additional function evaluations can improve the estimation procedure. Suppose that we obtain estimates $\xi_1, \xi_2, \dots, \xi_p$ corresponding to orthogonal vectors $z_1, z_2, \dots, z_q$ selected uniformly and randomly from the unit sphere S_{n-1}. The expected value of the norm of the projection of v onto the span $\mathcal{Z}$ generated by $z_1, z_2, \dots, z_q$ is

$$E\left(\sqrt{|z_1^T v|^2 + |z_2^T v|^2 + \dots + |z_q^T v|^2}\right) = \frac{W_n}{W_q}||v||\,.$$

The estimate $\nu(p) = \dfrac{W_q}{W_n}\sqrt{|z_1^T v|^2 + |z_2^T v|^2 + \dots + |z_q^T v|^2}$ is q-th order accurate, i.e., a relative error of size γ in the estimate occurs with probability proportional to γ^{-q}:

$$\Pr\left(\frac{||v||}{\gamma} \le \nu(q) \le \gamma||v||\right) \ge 1 - \frac{1}{p!}\left(\frac{2}{\pi\gamma}\right)^q + O\left(\frac{1}{\gamma^{q+1}}\right) \ .$$

3.1. SCE for estimation of approximation errors in model reduction. All error estimates derived in this paper begin with the linearizations of one of the ODEs (2.1), (2.3), (2.4) or perturbations of these. Thus the error estimates are based on solutions of linear error equations. To estimate the norm $\|e(t_f)\|$ of an error vector $e(t) \in R^n$ at $t = t_f$, we need to evaluate quantities $z_j^T e(t_f)$ for some random vector z_j selected uniformly from the unit sphere S_{n-1}. The norm estimate is then

$$||e(t_f)|| \approx \frac{W_q}{W_n} \sqrt{\sum_{j=1}^{q} |z_j^T e(t_f)|^2} \,. \tag{3.1}$$

The scalar products $z_j^T e(t_f)$ can be computed efficiently using an adjoint model (to the corresponding linear error equation) with final conditions at t_f based on the vector z_j. However, this approach naturally raises the question: *"What is the advantage of using (typically more than one) solution(s) of adjoint systems to estimate the norm of a quantity that can be otherwise obtained with only one forward ODE solution (of the error equation)?"* Our method is motivated by the fact that we are interested not only in finding the errors for one given ODE system, but rather in estimating (as efficiently as possible) the behavior of such errors for families of related ODE systems. In § 5 we study the concept of *regions of validity of reduced models*, i.e., the range of perturbations in the original ODE (2.1) over which the reduced model (2.3) is still appropriate. An approach based on forward error equations involves solving repeatedly such error equations (for each value of interest of the perturbation). On the other hand, an approach combining SCE estimates and adjoint models (as described in our paper) can be used to define what we term "condition numbers" for these error equations. While these condition numbers can provide only approximate upper bounds for the norms of the errors under investigation, they have the undeniable advantage of allowing *a-priori* estimates of the errors induced by perturbations, i.e., before having to solve such a perturbed system (or even a reduced perturbed system).

4. Estimation of the approximation error. We want to estimate the difference between the solution of the POD-reduced model (2.4) and the solution of the original equation (2.1). Let $\tilde{y}(t)$ be the projection onto S of the solution $y(t)$. The total approximation error $e(t) = \hat{y}(t) - y(t)$ can be split [20] into the subspace approximation error $e_\perp(t) = \tilde{y}(t) - y(t)$ and the error introduced by the integration in the subspace S, $e_i(t) = \hat{y}(t) - \tilde{y}(t)$:

$$e(t) = \hat{y}(t) - y(t) = (\hat{y}(t) - \tilde{y}(t)) + (\tilde{y}(t) - y(t)) = e_i(t) + e_\perp(t) \,. \tag{4.1}$$

The error component $e_\perp$ is orthogonal to S, while the component e_i is parallel to S (see Fig. 4.1). Algebraically, this is expressed as $Pe_\perp(t) = 0$ and $Pe_i(t) = e_i(t)$.

4.1. Total approximation error. Subtracting (2.1) from (2.4) yields an equation for the total error e

$$\begin{aligned}\frac{de}{dt} &= Pf(\hat{y},t) - f(y,t) = Pf(\hat{y},t) - f(\hat{y},t) + f(\hat{y},t) - f(y,t)\\ &= (P-I)f(\hat{y},t) - \mathbf{J}(\hat{y},t)(y-\hat{y}) + O(||e||^2)\,,\end{aligned}$$

where $\mathbf{J}$ is the Jacobian of the function f, i.e., $\mathbf{J} = \partial f/\partial y$. Let us introduce the notation $Q = I - P$. Thus, to a first order approximation, the error function satisfies

$$\frac{de}{dt} = \mathbf{J}(\hat{y},t)e(t) - Qf(\hat{y},t)\,, \quad e(t_0) = -Q(y_0 - \bar{y})\,. \tag{4.2}$$

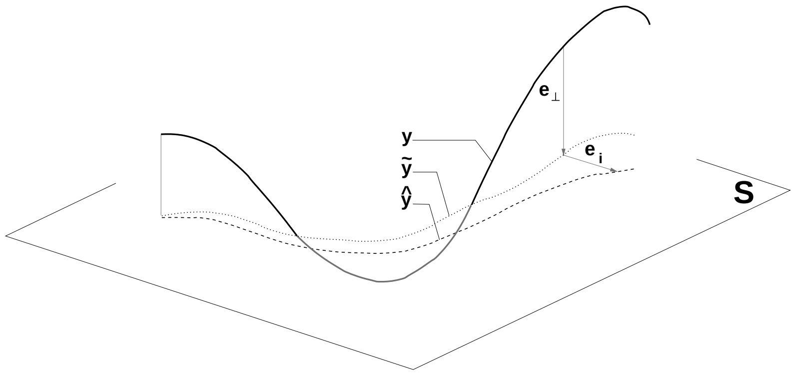


FIG. 4.1. *Solution and error components for POD-reduced models. y is the solution of the original ODE, $\tilde{y}$ is its projection on the affine subspace S, and $\hat{y}$ is the solution of the reduced model. The error component $e_\perp \in S^\perp$, while the subspace integration error component $e_i \in S$.*

Let the matrix function $\Phi_{\hat{y}}(t) \in R^{n\times n}$ satisfy

$$\frac{d\Phi_{\hat{y}}}{dt} = \mathbf{J}(\hat{y},t)\Phi_{\hat{y}}\,, \quad \Phi_{\hat{y}}(t_0) = I_n\,, \tag{4.3}$$

where the subscript $\hat{y}$ for $\Phi_{\hat{y}}$ indicates that the Jacobian is evaluated at $\hat{y}$. Then

$$e(t_f) = -\int_{t_0}^{t_f} \Phi_{\hat{y}}(t_f)\Phi_{\hat{y}}^{-1}(s)Qf(\hat{y}(s),s)\,ds - \Phi_{\hat{y}}(t_f)Q(y_0-\bar{y})\,.$$

For a random vector z uniformly selected from the unit sphere S_{n-1}, we have

$$z^T e(t_f) = -\int_{t_0}^{t_f} z^T\Phi_{\hat{y}}(t_f)\Phi_{\hat{y}}^{-1}(s)Qf(\hat{y}(s),s)\,ds - z^T\Phi_{\hat{y}}(t_f)Q(y_0-\bar{y})\,.$$

It is straightforward to verify that the solution $\lambda_{\hat{y}} \in R^n$ of the adjoint system

$$\frac{d\lambda_{\hat{y}}}{dt} = -\mathbf{J}^T(\hat{y},t)\lambda_{\hat{y}}\,, \quad \lambda_{\hat{y}}(t_f) = z \tag{4.4}$$

satisfies $\lambda_{\hat{y}}^T(s) = z^T\Phi(t_f)\Phi^{-1}(s)$ and $\lambda_{\hat{y}}^T(t_0) = z^T\Phi(t_f)$. As before, the subscript $\hat{y}$ indicates that the Jacobian in the adjoint system (4.4) is evaluated at $\hat{y}$. Therefore, the quantity $z^T e(t_f)$ is simply

$$z^T e(t_f) = -\int_{t_0}^{t_f} \lambda_{\hat{y}}^T(s)Qf(\hat{y}(s),s)\,ds - \lambda_{\hat{y}}^T(t_0)Q(y_0-\bar{y})\,. \tag{4.5}$$

The SCE estimate for the norm of $e(t_f)$ is obtained by combining (3.1) and (4.5)

$$||e(t_f)|| \approx \frac{W_q}{W_n}\sqrt{\sum_{j=1}^{q}\left|\int_{t_0}^{t_f} \lambda_{\hat{y}}^T(s)Qf(\hat{y}(s),s)\,ds + \lambda_{\hat{y}}^T(t_0)^TQ(y_0-\bar{y})\right|^2}\,. \tag{4.6}$$

The value of the integral is $\psi(t_0)$, where ψ satisfies the quadrature equation

$$\frac{d\psi}{dt} = -\lambda_{\hat{y}}^T(t)Qf(\hat{y}(t),t)\,, \quad \psi(t_f) = 0\,. \tag{4.7}$$

Algorithm 1 Estimate for the total approximation error

Provide the matrix of measurement data $\mathcal{Y}$
Set the POD dimension k
Compute mean value of data $\bar{y}$ and construct POD projection matrices ρ and P
Select (uniformly and randomly) q orthogonal vectors from the unit sphere S_{n-1}
Solve (2.3) for y^S
$\hat{y}(t) = \rho y^S(t) + \bar{y}$
Initialize $s = 0$
for $i = 1$ to q **do**
  Set $\lambda_{\hat{y}}(t_f) \leftarrow z_i$
  Solve (4.4)+(4.7) for $\lambda_{\hat{y}}$ and ψ
  Update $s \leftarrow s + \left[\psi(t_0) + \lambda_{\hat{y}}^T(t_0)^T Q(y_0 - \bar{y})\right]^2$
end for
Compute Wallis factors W_q and W_n
Compute the SCE norm estimate $e = (W_q/W_n) \times \sqrt{s}$

Algorithm 1 summarizes our approach.

It may seem more efficient to compute the SCE norm estimate using a POD-reduced adjoint system to evaluate $\lambda_{\hat{y}}$ in (4.6). Although the same projection can be used to model-reduce the adjoint system, this approach still requires knowledge of the mean of the adjoint solution, which is unavailable without a solution of the adjoint system (4.4). In other words, the approximation subspace S^λ is parallel to S but not identical to it. This issue can be circumvented if we are not considering error components outside the subspace S. This estimate is presented next. Its main advantage is given by the fact that the differential equations are solved in a space of dimension $k \ll n$, where n is the dimension of the solution for the original problem.

4.2. Subspace integration error. Differentiating $e_\perp(t) + e_i(t) = \hat{y}(t) - y(t)$ and substituting the ODEs for y and $\hat{y}$, we get

$$\frac{de_\perp}{dt} + \frac{de_i}{dt} = Pf(\hat{y}, t) - f(y, t)\,.$$

We project the above equation onto S (by multiplying on the left by P). Using that $Pe_\perp = 0$, we obtain an IVP for the subspace integration error:

$$\frac{de_i}{dt} = P\left(f(\hat{y}, t) - f(y, t)\right)\,, \quad e_i(t_0) = 0\,, \tag{4.8}$$

where we have used that $P^2 = P$. The starting point $\hat{y}(t_0)$ is the projection $\tilde{y}(t_0)$ of $y(t_0)$ onto S, yielding the initial condition $e_i(t_0) = 0$. Thus the subspace integration error is governed by an ODE with the subspace approximation error $e_\perp(t)$ as forcing term. An approximation to (4.8) is obtained by linearizing around the trajectory $\hat{y}(t)$:

$$\frac{de_i}{dt} = P\mathbf{J}(\hat{y}, t)e_i + P\mathbf{J}(\hat{y}, t)e_\perp\,, \quad e_i(t_0) = 0\,. \tag{4.9}$$

In the S coordinate system defined by the coordinate transformation

$$e_i^S = \rho^T e_i \in R^k\,, \qquad e_i \equiv \hat{e}_i = \rho e_i^S\,,$$

and using the identity $\rho^T\rho = I_k$, (4.9) can be written as

$$\frac{de_i^S}{dt} = \rho^T \mathbf{J}(\hat{y},t)\rho e_i^S + \rho^T \mathbf{J}(\hat{y},t) e_\perp \,, \quad e_i^S(t_0) = 0\,. \tag{4.10}$$

If $\phi_{\hat{y}} \in R^{k\times k}$ is the fundamental matrix, satisfying

$$\frac{d\phi_{\hat{y}}}{dt} = \rho^T \mathbf{J}(\hat{y},t)\rho\phi_{\hat{y}}\,, \quad \phi_{\hat{y}}(t_0) = I_k\,,$$

then, for a random vector z^S uniformly selected from the unit sphere S_{k-1}, we have

$$(z^S)^T e_i^S(t_f) = \int_{t_0}^{t_f} (z^S)^T \phi_{\hat{y}}(t_f)\phi_{\hat{y}}^{-1}(s)\rho^T \mathbf{J}(\hat{y}(s),s) e_\perp(s)\, ds\,.$$

Let $\mu_{\hat{y}}^T(s) = (z^S)^T\phi_{\hat{y}}(t_f)\phi_{\hat{y}}^{-1}(s)$, where $\mu_{\hat{y}}$ solves the adjoint system

$$\frac{d\mu_{\hat{y}}}{dt} = -\rho^T \mathbf{J}^T(\hat{y},t)\rho\mu_{\hat{y}}\,, \quad \mu_{\hat{y}}(t_f) = z^S \tag{4.11}$$

Therefore $(z^S)^T e_i^S(t_f) = \int_{t_0}^{t_f} \mu_{\hat{y}}^T(s)\rho^T\mathbf{J}(\hat{y}(s),s)e_\perp(s)\,ds$ and the SCE approximation for the norm of the subspace integration error is

$$||e_i(t_f)|| \approx \frac{W_q}{W_n}\sqrt{\sum_{j=1}^{q}\left|\int_{t_0}^{t_f} \mu_{\hat{y}}^T(s)\rho^T\mathbf{J}(\hat{y}(s),s)e_\perp(s)\,ds\right|^2}\,. \tag{4.12}$$

Bounds for the subspace integration error are obtained as follows. For some unit vector z_j^S in (4.11) let $\theta^j(s) = \mathbf{J}^T(\hat{y}(s),s)\rho_k\mu_{\hat{y}}(s) \in R^{N_y}$ and $w_j = \int_{t_0}^{t_f}(\theta^j)^T(s)e_\perp(s)\,ds$. Then

$$|w_j| \le \int_{t_0}^{t_f} |(\theta^j)^T(s)e_\perp(s)|\,ds \le \left(\int_{t_0}^{t_f}\sum_{i=1}^{N_y}|\theta_i^j(s)|\,ds\right)||e_\perp||_{L_\infty}\,. \tag{4.13}$$

Thus, defining $\kappa_j(e_i) = ||\theta^j||_{L_1} = \int_{t_0}^{t_f}\sum_{i=1}^{N_y}|\theta_i^j(s)|\,ds$, we have

$$||e_i(t_f)|| \le \kappa(e_i)\cdot||e_\perp||_{L_\infty}\,, \quad \kappa(e_i) = \frac{W_q}{W_n}\sqrt{\sum_{j=1}^{q}\kappa_j^2(e_i)}\,, \tag{4.14}$$

where $\kappa(e_i)$ can be seen as a "condition number" for the subspace integration error.

The expressions derived above require knowledge of the projection error $e_\perp$ at all times in $[t_0, t_f]$. While the projection error may not be readily available, its norm can be easily related to the error associated with the choice of the POD subspace. For this, a more convenient formulation of the POD approximation is to find a subspace $S \in R^n$ which minimizes the total square distance defined as

$$d^2 = \|\,(y-\bar{y}) - P\,(y-\bar{y})\,\|_{L_2}^2 = \int_{t_0}^{t_f}\|\,(y(s)-\bar{y}) - P\,(y(s)-\bar{y})\,\|_2^2\,ds\,. \tag{4.15}$$

The solution to this problem requires the construction of the correlation matrix

$$R = \int_{t_0}^{t_f}(y(s)-\bar{y})\,(y(s)-\bar{y})^T\;ds\,. \tag{4.16}$$

If $\lambda_1 \geq \ldots \geq \lambda_m \geq 0$ are the ordered eigenvalues of the symmetric positive semidefinite matrix R, then the minimum value of d^2 over all k-dimensional affine subspaces S passing through $\bar{y}$ is given by $\sum_{j=k+1}^{n} \lambda_j$. The minimizing S is the invariant subspace corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_k$, while the projection matrix ρ consists of the unit eigenvectors corresponding to these k largest eigenvalues. We also have that

$$||e_\perp||_{L_\infty} \leq ||e_\perp||_{L_2} \equiv \sqrt{\sum_{j=k+1}^{n} \lambda_j}\,.$$

Employing observations as data points for a trapezoidal approximation for the integral (4.15) leads to the same subspace S as the one obtained with the POD definition in §2, while the corresponding optimal total square distances will be proportional.

Finally, we note that, for a vector-valued function $f : [t_0, t_f] \to R^N$, the L_p norm ($p \geq 1$) is defined as

$$||f||_{L_p} = \left(\int_{t_0}^{t_f} ||f(s)||_p^p \, ds \right)^{1/p}, \text{ where } ||f(s)||_p = \left(\sum_{i=1}^{N} |f_i(s)|^p \right)^{1/p}.$$

In particular, $||f||_{L_1} = \int_{t_0}^{t_f} \sum_{i=1}^{N} |f_i(s)| \, ds$ and $||f||_{L_\infty} = \text{ess sup} \, (\max_i |f_i(s)|)$. With the above norm definitions, the inequality in (4.13) is just Hölder's inequality

$$||f^T g||_{L_1} \leq ||f||_{L_p} \cdot ||g||_{L_q}\,, \quad \text{if} \quad \frac{1}{p} + \frac{1}{q} = 1\,, \tag{4.17}$$

extended to vector-valued functions f and g, for $p = 1$ and $q = \infty$.

5. Regions of validity for POD-reduced models. Once a reduced model is constructed, we wish to apply it to simulate systems that are close in some sense to the system that was used for generating the reduced model. This raises the issue of defining the range of initial conditions and parameters over which the reduced model can be used with acceptable accuracy.

Let $Y \in R^n$ be the solution of an ODE obtained by applying a perturbation to (2.1), either in the initial conditions (in which case we use the notation Y^{ic}) or in the right-hand side (in which case we use the notation Y^{rhs}). Our goal is to estimate the errors introduced by this perturbation, in addition to the model reduction error $e(t)$. There are two perspectives from which this problem can be addressed.

Firstly, the reduced model might approximate the perturbed solution Y, given a POD projection matrix built using the solution of the unperturbed ODE (2.1). Then we want to estimate the error $E^1 = \hat{Y} - Y$, where $\hat{Y}$ is the solution of an ODE of the form (2.4), with P based on y. Alternatively, we may want estimates for the cumulative error (due to the POD model-reduction and the perturbation in the original ODE), $E^2 = \hat{Y} - y$, where $\hat{Y}$ is the solution of a POD reduced-model based on the solution Y of the perturbed ODE. Calculating $E^2 = \hat{Y} - y$ is completely equivalent to computing $E^2 = \hat{y} - Y$ (by considering y to be a perturbation to Y). To obtain SCE estimates for E_1 and E_2, we construct the ODE systems based on perturbations of the initial conditions

$$\frac{dY^{\text{ic}}}{dt} = f(Y^{\text{ic}}, t)\,, \quad Y^{\text{ic}}(t_0) = Y_0^{\text{ic}} = y_0 + \delta y_0\,, \tag{5.1}$$

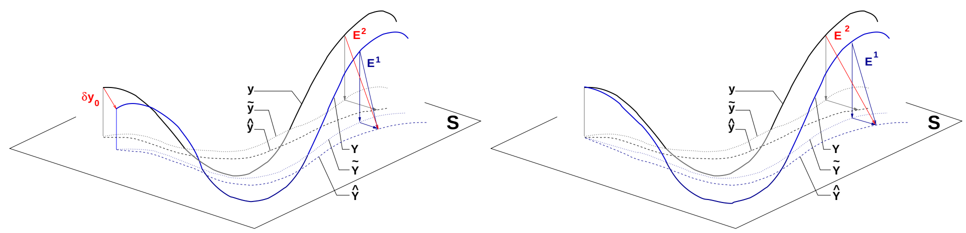
$$\frac{d\hat{Y}^{\text{ic}}}{dt} = P f(\hat{Y}^{\text{ic}}, t)\,, \quad \hat{Y}^{\text{ic}}(t_0) = P(Y_0^{\text{ic}} - \bar{y}) + \bar{y} \tag{5.2}$$

and on perturbations of right-hand side parameters

$$\frac{dY^{\text{rhs}}}{dt} = f(Y^{\text{rhs}}, t, p + \delta p)\,, \quad Y^{\text{rhs}}(t_0) = y_0\,, \tag{5.3}$$

$$\frac{d\hat{Y}^{\text{rhs}}}{dt} = Pf(\hat{Y}^{\text{rhs}}, t, p + \delta p)\,, \quad \hat{Y}^{\text{rhs}}(t_0) = P(y_0 - \bar{y}) + \bar{y}\,. \tag{5.4}$$

Figure 5.1 illustrates these solutions, as well as the errors e, E_1 and E_2.



(a) *Perturbation in initial conditions.* (b) *Perturbation in right-hand side.*

FIG. 5.1. *Error components in model-reduction of perturbed systems. The solution of the perturbed system, its projection onto S, and the solution of the reduced perturbed system are denoted by Y, $\tilde{Y}$, and $\hat{Y}$, respectively. The error E_1 represents the error committed in reducing the perturbed model, while E_2 is the cumulative error (perturbation + model-reduction).*

It is important to realize that *useful* estimates should not rely on the solution Y (or $\hat{Y}$) of the perturbed system (or its POD-reduction). Indeed, such error estimates are desired with the sole objective of deciding whether or not to solve these systems.

5.1. Estimation of $E^1_{\text{ic}} = \hat{Y}^{\text{ic}} - Y^{\text{ic}}$. An SCE estimate like (4.6) is not useful in the sense described above, as it would be based on the error equation

$$\frac{dE^1}{dt} = \mathbf{J}(\hat{Y}^{\text{ic}}, t)E^1 - Qf(\hat{Y}^{\text{ic}}, t)\,, \quad E^1(t_0) = -Q(y_0 + \delta y_0 - \bar{y})\,, \tag{5.5}$$

which is a linearization around the (unknown) trajectory $\hat{Y}^{\text{ic}}(t)$. Instead, let us define $\Delta^{\text{ic}}(t) = E^1(t) - e(t)$. The norm $\|E^1(t_f)\|$ can be bounded by

$$\Big|\|e(t_f)\| - \|\Delta^{\text{ic}}(t_f)\|\Big| \le \|E^1(t_f)\| \le \|e(t_f)\| + \|\Delta^{\text{ic}}(t_f)\|\,. \tag{5.6}$$

Any estimates of $\|\Delta^{\text{ic}}(t_f)\|$ would require solving the POD-reduced perturbed system (5.2). However, similar to §4.2, this problem can be circumvented by splitting the error Δ^{ic} into two components: $\Delta^{\text{ic}}_\perp$ orthogonal to S and Δ^{ic}_i parallel to S

$$\begin{aligned} \Delta^{\text{ic}} &= \Delta^{\text{ic}}_\perp + \Delta^{\text{ic}}_i\,, \quad \text{where} \\ \Delta^{\text{ic}}_\perp &= E^1_\perp - e_\perp = (\tilde{Y}^{\text{ic}} - Y^{\text{ic}}) - (\tilde{y} - y) = -Q(Y^{\text{ic}} - y) \\ \Delta^{\text{ic}}_i &= E^1_i - e_i = (\hat{Y}^{\text{ic}} - \tilde{Y}^{\text{ic}}) - (\hat{y} - \tilde{y}) = (\hat{Y}^{\text{ic}} - \hat{y}) - P(Y^{\text{ic}} - y) \end{aligned} \tag{5.7}$$

Next we evaluate the influence of δy_0 on each component separately. Retaining only the first order term of a Taylor series for $\Delta^{\text{ic}}_\perp$ around $\delta y_0 = 0$ and using the fact that $\Delta^{\text{ic}}_\perp = 0$ for $\delta y_0 = 0$, we get

$$\Delta^{\text{ic}}_\perp = -Q\left.\frac{dY^{\text{ic}}}{d\delta y_0}\right|_{\delta y_0 = 0} \delta y_0\,.$$

Differentiating (5.1) with respect to δy_0 leads to the sensitivity equation

$$\frac{d\Psi^{\rm ic}}{dt} = \mathbf{J}(y,t)\Psi^{\rm ic}\,, \quad \Psi^{\rm ic}(t_0) = I, \quad \text{where} \quad \Psi^{\rm ic} = dY^{\rm ic}/dy_0. \tag{5.8}$$

The Jacobian in (5.8) is evaluated at $\delta y_0 = 0$, in which case $Y^{\rm ic} \equiv y$. The sensitivity matrix $\Psi^{\rm ic}$ is the same as the fundamental matrix Φ_y corresponding to the ODE (2.1). For a uniformly selected random vector z, the solution λ_y of the adjoint system

$$\frac{d\lambda_y}{dt} = -\mathbf{J}^T(y,t)\lambda_y\,, \quad \lambda_y(t_f) = Qz\,, \quad z \in S_{n-1}\,, \tag{5.9}$$

combined with the fact that $Q^T = (I-P)^T = (I-P) = Q$, gives the equality

$$z^T\Delta_\perp^{\rm ic}(t_f) = z^T\left[-Q\Psi^{\rm ic}(t_f)\delta y_0\right] = -\lambda_y^T(t_0)\cdot\delta y_0\ . \tag{5.10}$$

Since $\Delta_\perp^{\rm ic}$ is orthogonal to S, a more accurate estimate can be obtained by using vectors from the sphere S_{n-k-1} embedded in $S^\perp$, instead of selecting vectors $z \in S_{n-1}$ and projecting them onto $S^\perp$, the orthogonal complement of S. If z' is the representation in R^n of such a vector, then $Qz' = z'$. The same adjoint system (5.9) and formula (5.10) can be used, but the probability that the estimate lies within a given factor w of the true norm $\|\Delta_\perp^{\rm ic}(t_f)\|$ is now higher (see note in §3). In practice we use the approximation $y \approx \hat{y}$ in evaluating the Jacobian in (5.9), with $\hat{y}$ computed from the solution y^S of the k-dimensional ODE (2.3).

Therefore, an SCE estimate of the norm of $\Delta_\perp^{\rm ic}(t_f)$ is given by

$$||\Delta_\perp^{\rm ic}(t_f)|| \approx \frac{W_q}{W_n}\sqrt{\sum_{j=1}^{q}|z'^T_j\Delta_\perp^{\rm ic}(t_f)|^2} = \frac{W_q}{W_n}\sqrt{\sum_{j=1}^{q}|\lambda_{\hat{y}}^T(t_0)\delta y_0|^2}\,, \tag{5.11}$$

where $\lambda_{\hat{y}}$ is the solution of $d\lambda_{\hat{y}}/dt = -\mathbf{J}^T(\hat{y},t)\lambda_{\hat{y}}$, $\lambda_{\hat{y}}(t_f) = Qz'_j$. Hölder's inequality (for $p = q = 2$) gives $|\lambda_{\hat{y}}^T(t_0)\delta y_0| \le ||\lambda_{\hat{y}}(t_0)||_2 \cdot ||\delta y_0||_2$, which implies

$$||\Delta_\perp^{\rm ic}(t_f)|| \le \kappa(\Delta_\perp^{\rm ic})\cdot||\delta y_0||\,, \tag{5.12}$$

where the "condition number" for the orthogonal component of $\Delta^{\rm ic}$ is defined as

$$\kappa(\Delta_\perp^{\rm ic}) = \frac{W_q}{W_n}\sqrt{\sum_{j=1}^{q}\kappa_j^2(\Delta_\perp^{\rm ic})}\,, \quad \kappa_j(\Delta_\perp^{\rm ic}) = ||\lambda_{\hat{y}}(t_0)||_2\,.$$

Differentiating with respect to time the expression for $\Delta_i^{\rm ic}$ in (5.7) and substituting the appropriate ODE right hand sides, we obtain first order approximations. The second of the following approximations is based on the assumption that $\mathbf{J}(y,t) \approx \mathbf{J}(\hat{y},t)$

$$\begin{aligned}\frac{d\Delta_i^{\rm ic}}{dt} &= \left(Pf(\hat{Y}^{\rm ic},t) - Pf(\hat{y},t)\right) - P\left(f(Y^{\rm ic},t) - f(y,t)\right)\\ &\approx P\mathbf{J}(\hat{y},t)(\hat{Y}^{\rm ic}-\hat{y}) - P\mathbf{J}(y,t)(Y^{\rm ic}-y) \approx P\mathbf{J}(\hat{y},t)\Delta_i^{\rm ic}\ .\end{aligned}$$

Since $E^1_{\mathbf{ic}}(t_0) = e_i(t_0) = 0$ it follows that $\Delta_i^{\rm ic}(t_0) = 0$ and, to a first order approximation, $\Delta_i^{\rm ic}(t) = 0$, for any $t \ge 0$. In other words, a perturbation to the initial conditions of the original ODE does not introduce additional subspace integration errors. As a consequence, $\Delta^{\rm ic}(t_f) \approx \Delta_\perp^{\rm ic}(t_f)$ and, combining (5.6) and (5.12), we have

$$\left| \|e(t_f)\| - \|\Delta_\perp^{\rm ic}(t_f)\| \right| \le \|E^1_{\bf ic}(t_f)\| \le \|e(t_f)\| + \kappa(\Delta_\perp^{\rm ic}) \cdot ||\delta y_0|| \,. \tag{5.13}$$

Note that, when using SCE estimates for the norms involved in the above bounds, the true value of $\|E^1_{\bf ic}(t_f)\|$ may not be bracketed by these bounds.

5.2. Estimation of $E^2_{\bf ic} = \hat{y} - Y^{\bf ic}$. Subtracting the ODEs satisfied by $\hat{y}$ and $Y^{\rm ic}$, the error $E^2_{\bf ic}$ satisfies, to a first order approximation,

$$\frac{dE^2_{\bf ic}}{dt} = {\bf J}(\hat{y},t)E^2_{\bf ic} - Qf(\hat{y},t)\,, \quad E^2_{\bf ic}(t_0) = -Q(y_0 - \bar{y}) - \delta y_0 \,. \tag{5.14}$$

For a uniformly selected random vector $z \in S_{n-1}$ and with $\lambda_{\hat{y}}$ the solution of (4.4), we have

$$\begin{aligned} z^T E^2(t_f) &= -\int_{t_0}^{t_f} \lambda_{\hat{y}}^T(s) Q f(\hat{y}(s),s)\, ds - \lambda_{\hat{y}}^T(t_0)\left(Q(y_0-\bar{y}) + \delta y_0\right) \\ &= z^T e(t_f) - \lambda_{\hat{y}}^T(t_0)\delta y_0 \,, \end{aligned} \tag{5.15}$$

where $e(t_f)$ is the approximation error for the original system, defined by (4.1). With the notation $\Gamma^{\rm ic}(t) = \Psi^{\rm ic}_{\hat{y}}(t)\delta y_0$ and combining (5.15) and (5.10), we conclude that

$$z^T E^2_{\bf ic}(t_f) = z^T \left[e(t_f) + \Gamma^{\rm ic}(t_f) \right] \,, \tag{5.16}$$

where $\Psi^{\rm ic}_{\hat{y}}$ is the solution of the IVP $d\Psi^{\rm ic}_{\hat{y}}/dt = {\bf J}(\hat{y},t)\Psi^{\rm ic}_{\hat{y}}$, $\Psi^{\rm ic}_{\hat{y}}(t_0) = I_n$. Thus, for $\lambda_{\hat{y}}$ the solution of (4.4), the following inequalities hold:

$$\left| \|e(t_f)\| - \|\Gamma^{\rm ic}(t_f)\| \right| \le \|E^2_{\bf ic}(t_f)\| \le \|e(t_f)\| + \kappa(\Gamma^{\rm ic}) \cdot ||\delta y_0|| \,, \tag{5.17}$$

where

$$||\Gamma^{\rm ic}(t_f)|| \approx \frac{W_q}{W_n} \sqrt{\sum_{j=1}^q |\lambda_{\hat{y}}^T(t_0)\delta y_0|^2} \quad \text{and} \quad \kappa(\Gamma^{\rm ic}) = \frac{W_q}{W_n} \sqrt{\sum_{j=1}^q \|\lambda_{\hat{y}}(t_0)\|_2^2} \,.$$

Since (5.16) holds for any vector z and final time t_f, we conclude that $E^2_{\bf ic} = e + \Gamma^{\rm ic}$, for any t. This implies that the SCE bound estimates (5.17) for the norm of $E^2_{\bf ic}(t_f)$ are more accurate than those derived in §5.1 for the norm of $E^1(t_f)$, based on the approximation $E^1 \approx e + \Delta_\perp^{\rm ic}$ (ignoring $\Delta_i^{\rm ic}$ and using $y \approx \hat{y}$ in the adjoint system). Furthermore, as seen from (5.15), an SCE estimate for $\|E^2_{\bf ic}(t_f)\|$ can be computed without need for $Y^{\rm ic}$ or $\hat{Y}^{\rm ic}$.

5.3. Estimation of $E^1_{\bf rhs} = \hat{Y}^{\bf rhs} - Y^{\bf rhs}$. Similar to §5.1, we decompose the error $\Delta^{\rm rhs} = E^1_{\bf rhs} - e$ into its components $\Delta_\perp^{\rm rhs} \in S^\perp$ and $\Delta_i^{\rm rhs} \in S$. We retain only the first order term from the Taylor expansion of $\Delta_\perp^{\rm rhs}$ around $\delta p = 0$

$$\Delta_\perp^{\rm rhs} = -Q \left. \frac{dY^{\rm rhs}}{d\delta p} \right|_{\delta p = 0} \delta p \,.$$

With $\Psi^{\rm rhs}$ the sensitivity matrix $dY^{\rm rhs}/dp$ and $\mathbf{K} = \partial f/\partial p$, we have

$$\frac{d\Psi^{\rm rhs}}{dt} = \mathbf{J}(y,t,p)\Psi^{\rm rhs} + \mathbf{K}(y,t,p)\,, \quad \Psi^{\rm rhs}(t_0) = 0\,,$$

The solution $\Psi^{\rm rhs}$ can be written in terms of the fundamental matrix Φ_y as

$$\Psi^{\rm rhs}(t_f) = \int_{t_0}^{t_f} \Phi_y(t_f)(\Phi_y(s))^{-1}\mathbf{K}(y(s),s,p)\,ds\ .$$

Using the solution λ_y of the adjoint system (5.9), we have, for an arbitrary $z \in R^n$

$$z^T\Delta_\perp^{\rm rhs}(t_f) = -\left(\int_{t_0}^{t_f} \lambda_y^T(s)\mathbf{K}(y(s),s,p)\,ds\right)\cdot\delta p\ . \tag{5.18}$$

The observations in §5.1 remain valid: (a) using vectors z' from the S_{n-k-1} sphere embedded in $S^\perp$ gives a more accurate SCE error norm estimate; and (b) a more efficient adjoint solution can be obtained assuming $\mathbf{J}(y,t,p) \approx \mathbf{J}(\hat{y},t,p)$ and $\mathbf{K}(y,t,p) \approx \mathbf{K}(\hat{y},t,p)$. Using (3.1) and (5.18), the SCE estimate of the norm of $\Delta_\perp^{\rm rhs}$ is

$$||\Delta_\perp^{\rm rhs}(t_f)|| \approx \frac{W_q}{W_n}\sqrt{\sum_{j=1}^q\left|\int_{t_0}^{t_f}\lambda_{\hat{y}}^T(s)\mathbf{K}(\hat{y}(s),s,p)\,\delta p\,ds\right|^2}\,, \tag{5.19}$$

bounded by $||\Delta_\perp^{\rm rhs}(t_f)|| \le \kappa(\Delta_\perp^{\rm rhs})\cdot||\delta p||_\infty$, where $\kappa(\Delta_\perp^{\rm rhs})$ is defined as

$$\kappa(\Delta_\perp^{\rm rhs}) = \frac{W_q}{W_n}\left[\sum_{j=1}^q \kappa_j^2(\Delta_\perp^{\rm rhs})\right]\,, \quad \kappa_j(\Delta_\perp^{\rm rhs}) = ||\lambda_{\hat{y}}^T\mathbf{K}||_{L_1}\,.$$

With $\mathbf{K}$ defined as above, the component $\Delta_i^{\rm rhs}$ parallel to S satisfies the ODE

$$\begin{aligned}\frac{d\Delta_i^{\rm rhs}}{dt} &= \left(Pf(\hat{Y}^{\rm rhs},t,p+\delta p) - Pf(\hat{y},t,p)\right) - P\left(f(Y^{\rm rhs},t,p+\delta p) - f(y,t,p)\right)\\ &\approx P\left(\mathbf{J}(\hat{y},t,p)(\hat{Y}^{\rm rhs}-\hat{y}) + \mathbf{K}(\hat{y},t,p)\,\delta p\right) - P\left(\mathbf{J}(y,t)(Y^{\rm rhs}-y) + \mathbf{K}(y,t,p)\,\delta p\right)\ .\end{aligned}$$

Using the approximations $\mathbf{J}(y,t,p) \approx \mathbf{J}(\hat{y},t,p)$ and $\mathbf{K}(y,t,p) \approx \mathbf{K}(\hat{y},t,p)$, we obtain

$$\frac{d\Delta_i^{\rm rhs}}{dt} = P\mathbf{J}(\hat{y},t,p)\Delta_i^{\rm rhs}\,.$$

Since $\Delta_i^{\rm rhs}(t_0) = 0$ it follows that, to a first order approximation, $\Delta_i^{\rm rhs}(t) = 0$, for any $t \ge 0$. As a consequence, $\Delta^{\rm rhs}(t_f) \approx \Delta_\perp^{\rm rhs}(t_f)$ and therefore

$$\Big|\|e(t_f)\| - \|\Delta_\perp^{\rm rhs}(t_f)\|\Big| \;\le\; \|E^1_{\mathbf{rhs}}(t_f)\| \;\le\; \|e(t_f)\| + \kappa(\Delta_\perp^{\rm rhs})\cdot||\delta p||_\infty\,. \tag{5.20}$$

5.4. Estimation of $E^2_{\mathbf{rhs}} = \hat{y} - Y^{\mathbf{rhs}}$. Following a similar approach to §5.3, for a uniformly selected random vector $z \in S_{n-1}$ and with $\lambda_{\hat{y}}$ the solution of (4.4)

$$\begin{aligned} z^T E^2(t_f) &= -\int_{t_0}^{t_f} \lambda_{\hat{y}}^T(s)\left[Qf(\hat{y}(s),s,p) + \mathbf{K}(\hat{y}(s),s,p)\,\delta p\right] ds \\ &\qquad - \lambda_{\hat{y}}^T(t_0)Q(y_0 - \bar{y}) \\ &= z^T e(t_f) - \int_{t_0}^{t_f} \lambda_{\hat{y}}^T(s)\mathbf{K}(\hat{y}(s),s,p)\,\delta p\, ds\,, \end{aligned} \tag{5.21}$$

where $e(t_f)$ is the approximation error for the original system, defined by (4.1). As in §5.2, we can write $E^2_{\mathbf{rhs}} = e + \Gamma^{\mathrm{rhs}}$, with $\Gamma^{\mathrm{rhs}}(t) = \Psi_{\hat{y}}^{\mathrm{rhs}}(t)\,\delta p$ and

$$\frac{d\Psi_{\hat{y}}^{\mathrm{rhs}}}{dt} = \mathbf{J}(\hat{y},t,p)\Psi_{\hat{y}}^{\mathrm{rhs}} + \mathbf{K}(\hat{y},t,p)\,, \quad \Psi_{\hat{y}}^{\mathrm{rhs}}(t_0) = 0\,.$$

Therefore, using $\|\Gamma^{\mathrm{rhs}}(t_f)\| \le \|\delta p\|_\infty$, the following inequalities hold:

$$\Big| \|e(t_f)\| - \|\Gamma^{\mathrm{rhs}}(t_f)\| \Big| \;\le\; \|E^2_{\mathbf{rhs}}(t_f)\| \;\le\; \|e(t_f)\| + \kappa(\Gamma^{\mathrm{rhs}}) \cdot \|\delta p\|_\infty\,. \tag{5.22}$$

With $\lambda_{\hat{y}}$ the solution of (4.4), the quantities in the above expression are

$$\begin{aligned} ||\Gamma^{\mathrm{rhs}}(t_f)|| &\approx \frac{W_q}{W_n}\sqrt{\sum_{j=1}^{q}\left|\int_{t_0}^{t_f} \lambda_{\hat{y}}^T(s)\mathbf{K}(\hat{y}(s),s,p)\,\delta p\, ds\right|^2} \\ \text{and} \quad \kappa(\Gamma^{\mathrm{rhs}}) &= \frac{W_q}{W_n}\sqrt{\sum_{j=1}^{q} \|\lambda_{\hat{y}}^T \mathbf{K}\|_{L_1}^2} \end{aligned}$$

The above SCE bound estimates for the norm of $E^2_{\mathbf{rhs}}(t_f)$ are more accurate than those derived in §5.3 for the norm of $E^1_{\mathbf{rhs}}(t_f)$. Furthermore, starting from (5.21), an SCE estimate for $\|E^2_{\mathbf{rhs}}(t_f)\|$ can be computed without need for Y^{rhs} or $\hat{Y}^{\mathrm{rhs}}$.

6. Examples. We consider reduced-order ODE examples that are representative of problems derived from spatial discretization of PDEs (linear advection-diffusion) or directly obtained from physical phenomena (a pollution model). Additional examples are described in [9]. For each example, two figures with numerical results are provided (Figs. 6.2 and 6.3 for the first example and in Figs. 6.5 and 6.6 for the second one.) The estimates (and bounds) were obtained using $N_z = 1$ (blue), $N_z = 2$ (green), and $N_z = 3$ (red), where N_z is the number of orthogonal vectors used by the SCE.

The first figure contains POD approximation errors as functions of the dimension of the subspace S. The norm of the total approximation error at the final time, $\|e(t_f)\| = \|\hat{y}(t_f) - y(t_f)\|$, is given in plot ($a$), while the norm of the subspace integration error at the final time, computed in the subspace S, i.e., $\|e_i^S(t_f)\|$ is presented in plot (b). The solid (black) lines represent the corresponding norms computed by the forward integration of the error equations (4.2) and (4.10), respectively. The dotted (colored) lines describe SCE estimates (4.6) and (4.12), respectively, for different values of q. The dashed (colored) lines appear only in plot (b) and represent the bounds of (4.14) for different values of q.

The first four plots in the second figure contain estimates of errors induced by a perturbation δy_0 in the initial conditions. Plot (a) presents the norm of the total approximation error of the perturbed system at the final time, $\|E^1(t_f)\| = \|\hat{Y}^{\mathrm{ic}}(t_f) - Y^{\mathrm{ic}}(t_f)\|$, as a function of the subspace dimension N_k. Plot (b) contains the norm of the cumulative error of the perturbed system at the final time, $\|E^2(t_f)\| = \|\hat{y}(t_f) - Y^{\mathrm{ic}}(t_f)\|$, as a function of the subspace dimension N_k. Plots (c) and (d) present the error bounds for $\|E^1_{\mathbf{ic}}(t_f)\|$ and $\|E^2_{\mathbf{ic}}(t_f)\|$, respectively, as predicted by the condition number $\kappa(\Delta^{\mathrm{ic}}_{\perp})$ over a range of perturbations δy_0, for a given value of N_k. The solid (black) line represents the norm computed by the forward integration of the error equations (5.5) and (5.14), respectively. For different values of q, the dashed (colored) lines represent SCE estimates of the upper bound of (5.13) in plots (a) and (b), and of (5.17) in plots (c) and (d). For different values of q, the dotted (colored) lines represent SCE estimates for $\|E^1_{\mathbf{ic}}(t_f)\|$ in plot (a) and for $\|E^2_{\mathbf{ic}}(t_f)\|$ in plot (b).

The last four plots in the second figure contain estimates of errors induced by a perturbation δp in the model parameters. The corresponding plots (e), (f), (g), and (h) are in a format which is analogous to the one above.

The (blue) line made of circles represents the norm of the "exact error", $e(t) = \hat{y}(t) - y(t)$, where $\hat{y}$ is the solution of (2.4) and y is the solution of (2.1).

Dimension of the POD subspace. Let $\Lambda_k = \sum_{i=k+1}^{n} \lambda_i$ be the sum of the eigenvalues ignored in the construction of the POD reduced model and $\Lambda = \Lambda_k / \sum_{i=1}^{n} \lambda_i$ be its relative size compared to the sum of all eigenvalues. The POD subspace dimension k is selected such that the relative error is very close to one, yet k is sufficiently small. A relative error near zero means that a high percentage of the energy for the full model was captured by the reduced order model. The values of Λ_k and Λ, for the numerical examples considered in this paper, are presented in Table 6.1.

TABLE 6.1
The sum of ignored eigenvalues Λ_k and their relative size Λ

	Example 1: Advection diffusion		Example 2: Pollution model	
N_k	Λ_k	Λ	Λ_k	Λ
5	1.803561e-01	5.890413e-06	6.341930e-13	2.652438e-12
6	2.831234e-02	9.246781e-07	6.971282e-14	2.915657e-13
7	4.193422e-03	1.369567e-07	1.139176e-15	4.764470e-15
8	5.662276e-04	1.849294e-08	1.175776e-16	4.917547e-16
9	6.944298e-05	2.268001e-09	4.938977e-17	2.065669e-16
10	7.716002e-06	2.520038e-10	9.158667e-18	3.830506e-17

An interesting phenomenon can be observed in some of the numerical experiments. Some of the estimates computed for a certain number of POD vectors are not as good as estimates corresponding to a smaller POD subspace dimension. At first glance this would contradict the theoretical description of the POD method, which implies that the original model would be better approximated as the POD dimension increases. In fact there is no contradiction. If one considers the entire time interval, one can notice that the reduced model captures a larger percentage of the original problem as we add more POD vectors. But our figures show the behavior of the reduced model only at the final time, not over the entire time interval.

Number of orthogonal vectors for the SCE estimate. We considered one, two, and three SCE vectors for our numerical examples. As expected, having just one SCE vector yielded the worst estimate in most of the cases. Nevertheless, even that estimate was, in many cases, "close enough" to warrant its inclusion in our results.

6.1. Linear advection-diffusion model. We consider the 1-D problem

$$\begin{aligned} & u_t = p_1 u_{xx} + p_2 u_x \\ \text{with B.C.} \quad & u(0,t) = u(2,t) = 0 \\ \text{and I.C.} \quad & u(x,0) = u_0(x) = x(2-x)e^{2x} \,. \end{aligned}$$

The PDE is discretized on a uniform grid of size $N+2$ with central differencing. With $y_i(t) = u(x_i,t)$ and eliminating boundary values, we obtain a size N ODE system

$$\frac{dy_i}{dt} = p_1 \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} + p_2 \frac{y_{i+1} - y_{i-1}}{2\Delta x} \,, \quad y_i(0) = u_0(x_i) \,.$$

The problem parameters were $p_1 = 0.5$, $p_2 = 1.0$ and $N = 100$. The solution behavior and numerical results are shown in Fig. 6.1, respectively in Figs. 6.2 and 6.3. The POD projection matrices were based on $m = 100$ data points equally spaced in the interval $[t_0, t_f] = [0.0, 0.3]$. The estimate of the total error is consistently "close" to the exact value, with the estimates corresponding to $N_z = 2, 3$ almost identical to the subspace integration error. The bounds are within an order of magnitude for both IC and RHS perturbations. The RHS perturbation increases the distance between the bounds and the forward error. That was expected, since the RHS perturbation changes the advection coefficient p_2, which is dominant for the time window considered.

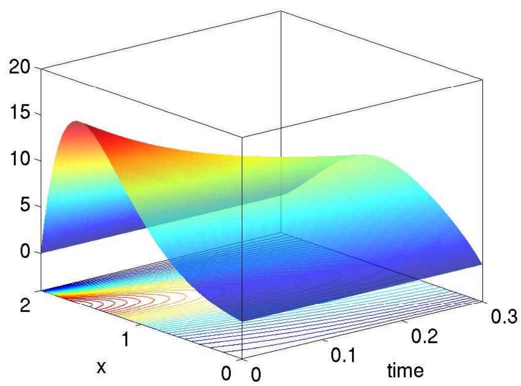
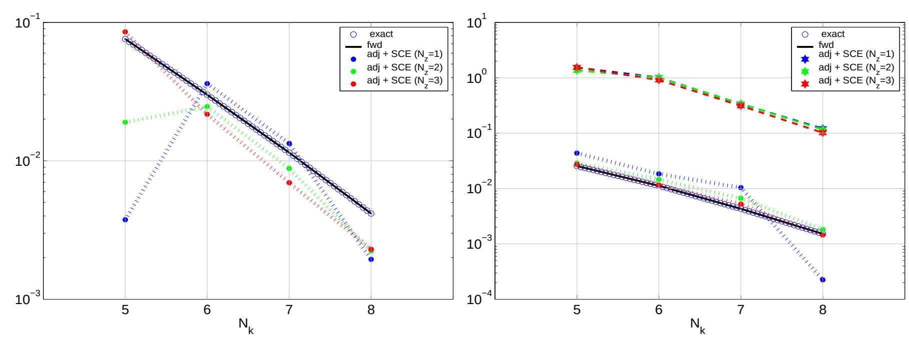
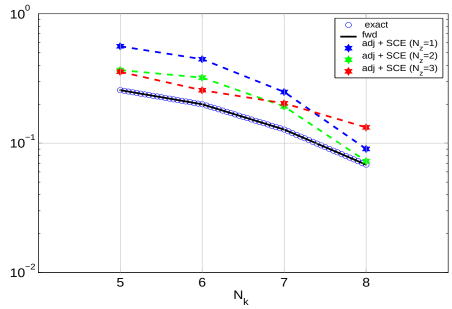


FIG. 6.1. *1D advection-diffusion example. Behavior of the solution over the integration interval.*

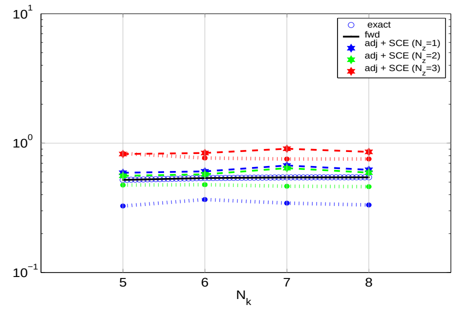


(a) *Total error* (b) *Subspace integration error*

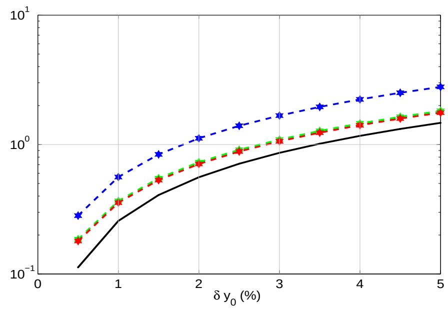
FIG. 6.2. *1D advection-diffusion example. Approximation error.*



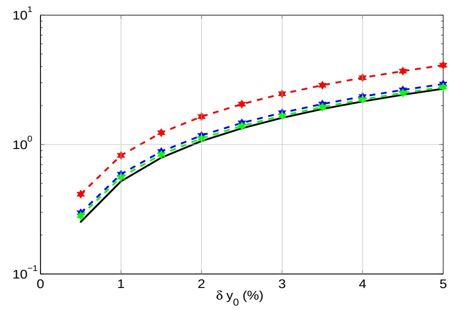
(a) *Approximation error* E^1 *as function of the subspace dimension (*$\delta y_0 = 1.0\%$*)*



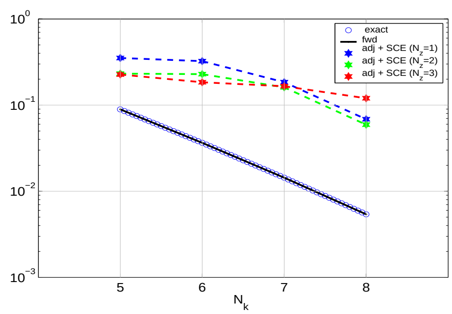
(b) *Cumulative error* E^2 *as function of the subspace dimension (*$\delta y_0 = 1.0\%$*)*



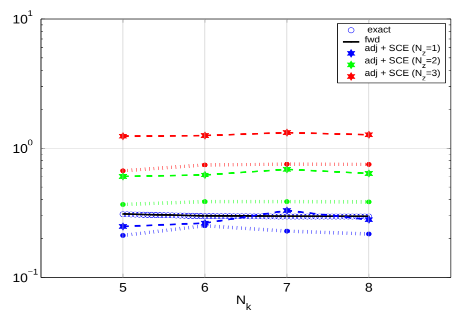
(c) *Approximation error* E^1 *as function of the IC perturbation (*$N_k = 5$*)*



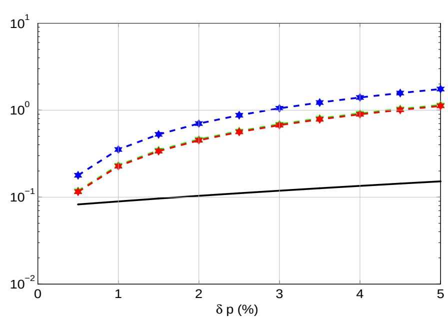
(d) *Cumulative error* E^2 *as function of the IC perturbation (*$N_k = 5$*)*



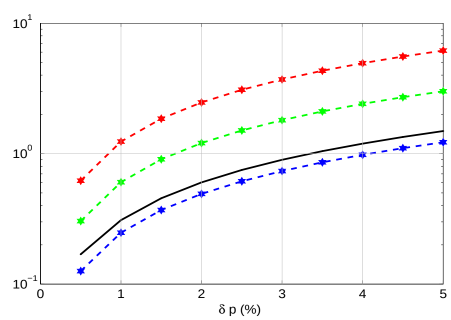
(e) *Approximation error* E^1 *as function of the subspace dimension (*$\delta p = 1.0\%$*)*



(f) *Cumulative error* E^2 *as function of the subspace dimension (*$\delta p = 1.0\%$*)*



(g) *Approximation error* E^1 *as function of the RHS perturbation (*$N_k = 5$*)*



(h) *Cumulative error* E^2 *as function of the RHS perturbation (*$N_k = 5$*)*

FIG. 6.3. *1D advection-diffusion example. Regions of validity.*

6.2. Pollution model. Next we consider the chemical reactions from an air pollution model described in [26]. It is a highly stiff ODE system consisting of 25 reactions and 20 species. The problem is of the form

$$\frac{dy}{dt} = f(y)\,, \quad y(0) = y_0, \quad y \in R^{20}\ ,$$

where the function $f(y)$ is defined by

$f_1 = -\sum_{j\in\{1,10,14,23,24\}} r_j + \sum_{j\in\{2,3,9,11,12,22,25\}} r_j$ $\quad f_{12} = r_9$
$f_2 = -r_2 - r_3 - r_9 - r_{12} + r_1 + r_{21}$ $\quad f_{14} = -r_{13} + r_{12}$
$f_3 = -r_{15} + r_1 + r_{17} + r_{19} + r_{22}$ $\quad f_{18} = r_{20}$
$f_4 = -r_2 - r_{16} - r_{17} - r_{23} + r_{15}$ $\quad f_{13} = -r_{11} + r_{10}$
$f_5 = -r_3 + r_4 + r_4 + r_6 + r_7 + r_{13} + r_{20}$ $\quad f_{17} = -r_{20}$
$f_6 = -r_6 - r_8 - r_{14} - r_{20} + r_3 + 2r_{18}$ $\quad f_{15} = r_{14}$
$f_7 = -r_4 - r_5 - r_6 + r_{13}$ $\quad f_{16} = -r_{18} - r_{19} + r_{16}$
$f_8 = r_4 + r_5 + r_6 + r_7$ $\quad f_{10} = -r_{12} + r_7 + r_9$
$f_{11} = -r_9 - r_{10} + r_8 + r_{11}$ $\quad f_9 = -r_7 - r_8$
$f_{19} = -r_{21} - r_{22} + r_{22} - r_{24} + r_{25}$ $\quad f_{20} = -r_{25} + r_{24}$

and $y_0 = [0, 0.2, 0, 0.04, 0, 0, 0.1, 0.3, 0.01, 0.0, 0, 0, 0, 0, 0, 0.007, 0, 0, 0]^T$. The auxiliary variables r_j and the model parameters k_j are given in Table 6.2. Figure 6.4 presents the solution behavior over the integration domain. Numerical results depicting the

TABLE 6.2
Auxiliary variables (r_j) and model parameters (k_j) for the pollution model

$r_1 = k_1 y_1$	$r_7 = k_7 y_9$	$r_{13} = k_{13} y_{14}$	$r_{19} = k_{19} y_{16}$
$r_2 = k_2 y_2 y_4$	$r_8 = k_8 y_9 y_6$	$r_{14} = k_{14} y_1 y_6$	$r_{20} = k_{20} y_{17} y_6$
$r_3 = k_3 y_5 y_2$	$r_9 = k_9 y_{11} y_2$	$r_{15} = k_{15} y_3$	$r_{21} = k_{21} y_{19}$
$r_4 = k_4 y_7$	$r_{10} = k_{10} y_{11} y_1$	$r_{16} = k_{16} y_4$	$r_{22} = k_{22} y_{19}$
$r_5 = k_5 y_7$	$r_{11} = k_{11} y_{13}$	$r_{17} = k_{17} y_4$	$r_{23} = k_{23} y_1 y_4$
$r_6 = k_6 y_7 y_6$	$r_{12} = k_{12} y_{10} y_2$	$r_{18} = k_{18} y_{16}$	$r_{24} = k_{24} y_{19} y_1$
			$r_{25} = k_{25} y_{20}$
$k_1 = 0.350 \cdot 10^0$	$k_7 = .130 \cdot 10^{-3}$	$k_{13} = .188 \cdot 10^1$	$k_{19} = .444 \cdot 10^{12}$
$k_2 = 0.266 \cdot 10^2$	$k_8 = .240 \cdot 10^5$	$k_{14} = .163 \cdot 10^5$	$k_{20} = .124 \cdot 10^4$
$k_3 = .123 \cdot 10^5$	$k_9 = .165 \cdot 10^5$	$k_{15} = .480 \cdot 10^7$	$k_{21} = .210 \cdot 10^1$
$k_4 = .860 \cdot 10^{-3}$	$k_{10} = .900 \cdot 10^4$	$k_{16} = .350 \cdot 10^{-3}$	$k_{22} = .578 \cdot 10^1$
$k_5 = .820 \cdot 10^{-3}$	$k_{11} = .220 \cdot 10^{-1}$	$k_{17} = .175 \cdot 10^{-1}$	$k_{23} = .474 \cdot 10^{-1}$
$k_6 = .150 \cdot 10^5$	$k_{12} = .120 \cdot 10^5$	$k_{18} = .100 \cdot 10^9$	$k_{24} = .178 \cdot 10^4$
			$k_{25} = .312 \cdot 10^1$

approximation errors and the regions of validity at $t_f = 1.0$ are presented in Figs. 6.5 and 6.6, respectively. The POD projection matrix was based on $m = 1000$ data points equally spaced in the interval $[t_0, t_f] = [0.0, 1.0]$. For $N_k = 5, 6, 7$ the total error and the subspace integration error are very well approximated by estimates corresponding to $N_z = 2$ or 3. For $N_k = 8, 9, 10$ the estimates are not as good, although they remain within an order of magnitude. We believe that this behavior is related to the fact that the POD error (either absolute or relative) is very small. We note that the problem was solved using tolerances of $rtol = 10^{-4}$ and $atol = 10^{-7}$. Thus one can expect a less uniform behavior if the results are in the neighborhood of 10^{-7}.

Finally, we note that, due to the fact that the problem parameters k_j have orders of magnitude ranging from 10^{-3} to 10^{12}, we have limited the RHS perturbation only to perturbations in k_4, k_5, and k_7.

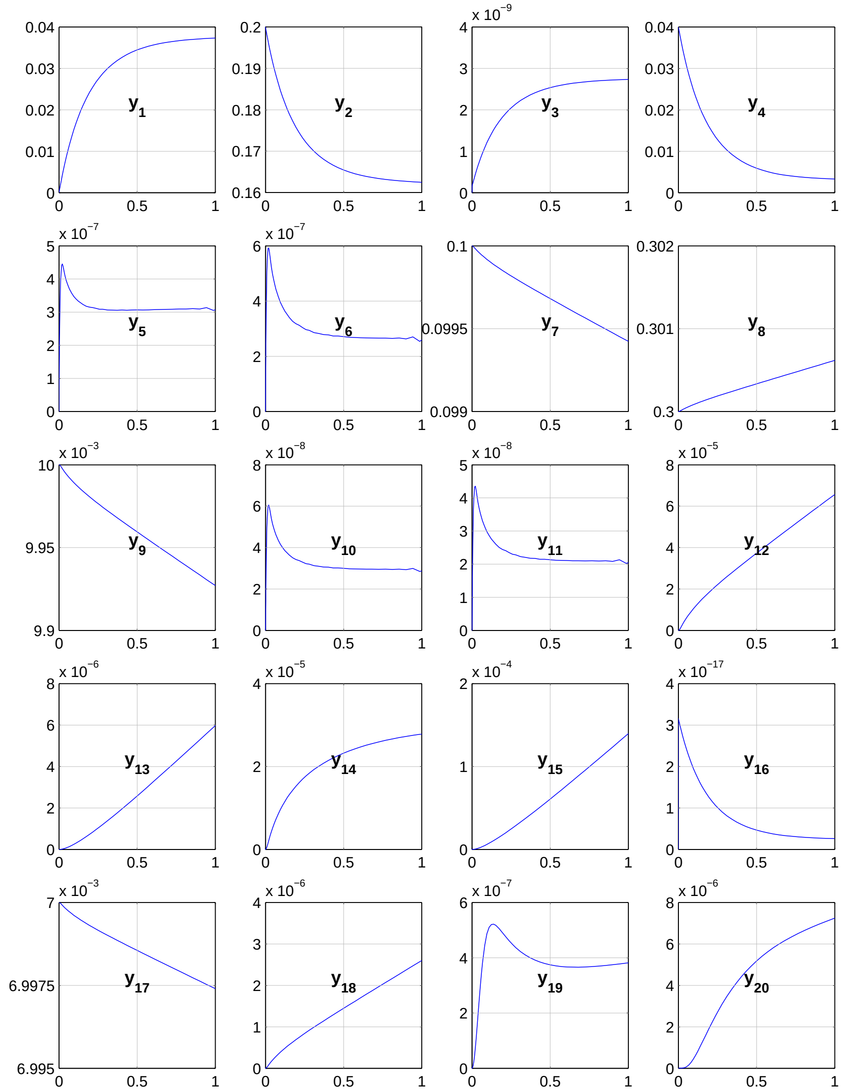
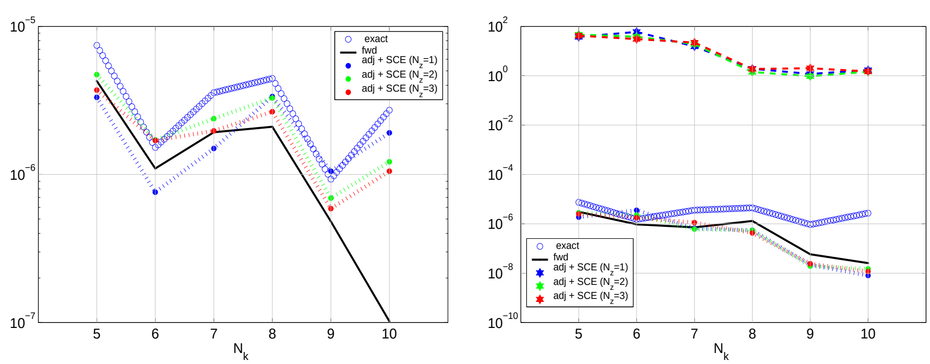
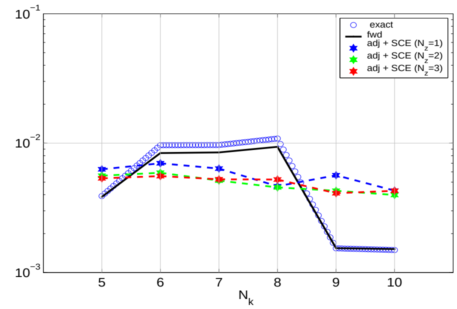


FIG. 6.4. *Pollution example. Behavior of the solution over the integration interval.*

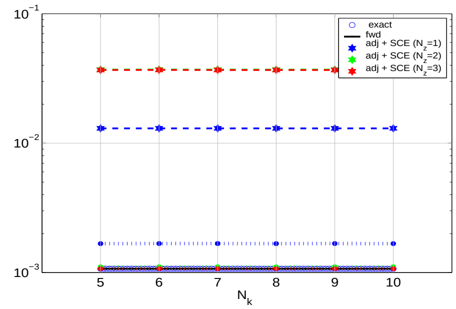


(a) *Total error* (b) *Subspace integration error*

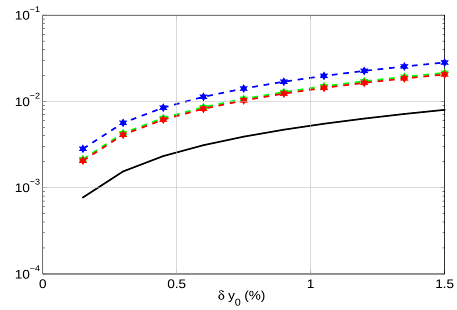
FIG. 6.5. *Pollution example. Approximation error.*



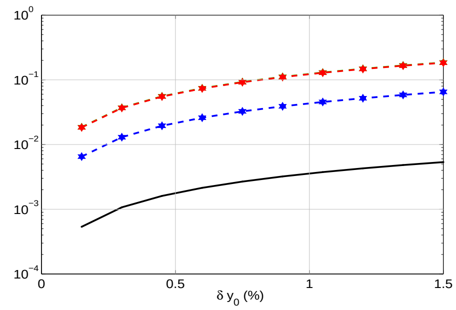
(a) *Approximation error E^1 as function of the subspace dimension ($\delta y_0 = 0.3\%$)*



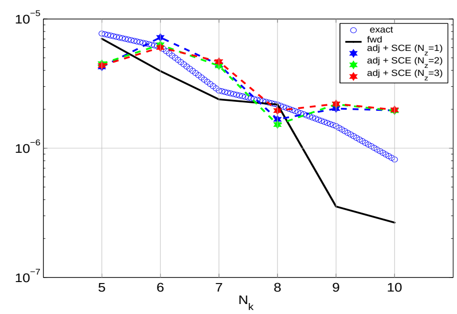
(b) *Cumulative error E^2 as function of the subspace dimension ($\delta y_0 = 0.3\%$)*



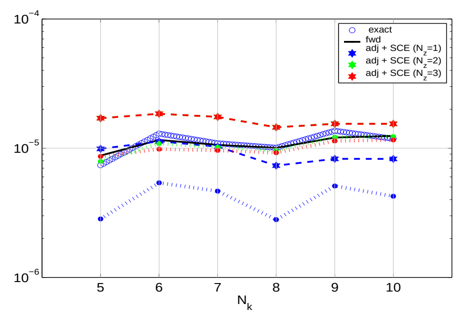
(c) *Approximation error E^1 as function of the IC perturbation ($N_k = 5$)*



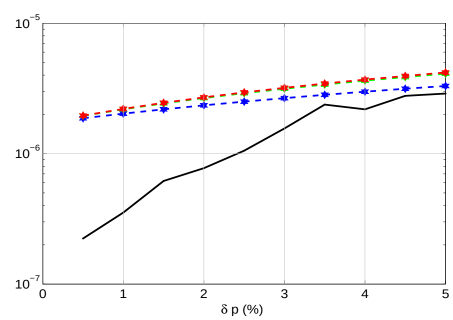
(d) *Cumulative error E^2 as function of the IC perturbation ($N_k = 5$)*



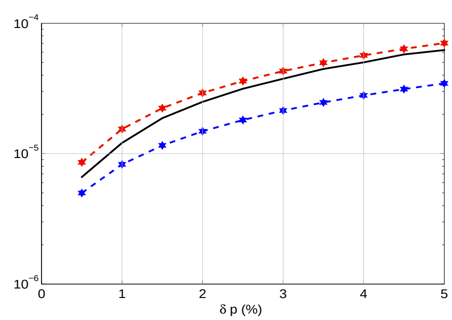
(e) *Approximation error E^1 as function of the subspace dimension ($\delta p = 1.0\%$)*



(f) *Cumulative error E^2 as function of the subspace dimension ($\delta p = 1.0\%$)*



(g) *Approximation error E^1 as function of the RHS perturbation ($N_k = 5$)*



(h) *Cumulative error E^2 as function of the RHS perturbation ($N_k = 5$)*

FIG. 6.6. *Pollution example. Regions of validity.*

7. Conclusions and Future Work. We have presented effective methods for estimating approximation errors due to the use of POD-based reduced order models and for evaluating regions of validity of such reduced models. The bounds defining these regions of validity are *a-priori*, in the sense that they do not rely on the solution of the perturbed system. The proposed approach, based on SCE norm estimates combined with the adjoint method, allows the definition and construction of so-called "error condition numbers" which can be used to assess the size of errors induced by perturbations (in initial conditions or in the model itself) without having to solve the perturbed system. The effectiveness of the proposed methods was demonstrated on several test problems.

In future work, we plan to investigate the applicability of this technique to the estimation of errors from other types of reduced order models.

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