Short note

Uncertain data in initial boundary value problems: Impact on short and long time predictions

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Abstract

We investigate the influence of uncertain data on solutions to initial boundary value problems with well posed boundary conditions. Uncertainty in the forcing function, initial conditions and boundary conditions are considered and we quantify their relative influence for short and long time calculations. For short time calculations, uncertainty in the initial data dominates. As time grows, the influence of initial data vanishes exponentially fast. For longer time calculations, the uncertainty in the forcing function and boundary data dominate, as they grow in time. Errors due to the forcing function grow faster (linearly in time) than the ones due to the boundary data (grow as the square root of time). Roughly speaking, the results indicate that for short time calculations, the initial conditions are the most important, but for longer time calculations, focus should be on the forcing function and boundary conditions. The findings are especially important when similar mathematical and numerical techniques are used for both short and long times. Our qualitative results can guide more quantitative investigations where details of the uncertain data are known.

1. Introduction

Approximative solutions which constitute the output to initial boundary value problems (IBVPs) are for most applications of practical interest generated by numerical algorithms such as finite difference [1–3], finite volume [4,5], spectral elements [6,7], flux reconstruction [8,9], discontinuous Galerkin [10–12] and continuous Galerkin [13,14] schemes. The investigation of stability, accuracy and convergence of these approximations dominate in the numerical analysis literature (see [15–21] for examples regarding linear problems and [22–30] for nonlinear ones). However, no output can be better than the quality of the input, which for IBVPs consists of forcing functions, initial data and boundary data (irrespectively of the preferred scheme). This fact has historically attracted less interest and often the quality of the data is assumed to be high enough. However, that the quality of the input data may be problematic have also been realised e.g. in aerospace [31–33], nuclear physics [34,35], oil prospecting [36–39], weather forecasts [40–42] and climate predictions [43–46] to name a few.

The main motivation for this work was the different views on external input in applications where otherwise similar computational technology is used. In aeronautical flow investigations using computational fluid dynamics (CFD) for example, some solutions (e.g. steady state and flutter solutions) are obtained by long time integration and the initial data is often ignored (being typically an arbitrary constant). The specifics of the solution is assumed to be given by the governing equations combined with boundary
conditions and the IBVP is essentially viewed as a boundary value problem (BVP). This view is quite different from the one in numerical weather prediction (NWP), where creating appropriate initial data for ensemble predictions [47] and data assimilation is very important. These procedures together with ingesting available observational data provide the NWP prediction with the character of an initial value problem (IVP). Both in CFD and NWP various modelling efforts include parameter values describing effects not completely known. In CFD those are present in turbulence models [48] and shock treatments [49]. For NWP they are employed in models for cloud formation, rainfall, and various transport phenomena [50]. Appropriate choices of these parameters in the governing equations are necessary for successful predictions and the uncertainty can be described by the forcing function.

In many of the application areas above, so called uncertainty quantification (UQ) has been used to address the problem [51–56]. The forward propagation procedure can roughly be described as: given a certain input with a probability distribution, how can its influence on the statistically distributed output be estimated? The inverse procedure (data assimilation) can roughly be described as: how can the appropriate statistical input be arranged such that a reasonable correct statistical output is obtained? The medium-range forecasting is accompanied by ensemble predictions using lower resolution than the deterministic forecast but a set of numerous concomitant simulations with differently perturbed initial conditions.

The UQ approach is pragmatic, informative and rather technical in nature but sometimes disregards fundamental properties of the governing IBVP (although exceptions exist [56–58]).

In this paper, we will proceed differently and focus on the fundamental IBVP properties. We will employ previous knowledge about IBVPs used in so called error bounded schemes [59–61]. These schemes use well posed boundary conditions that generate a damping term in the energy rate that subsequently lead to error bounds. We will in addition use the recent development for IBVPs in [62–64] where it is shown that an energy bound of both the nonlinear and linearised IBVP can be obtained if a skew-symmetric form of the governing equations is available. We will combine the techniques mentioned above and study the effects of errors in the forcing function, initial data and boundary data on the solution. Our qualitative analysis of the response to uncertain data may guide a more quantitative analysis in specific cases using UQ.

The results from the continuous analysis roughly described above hold also for numerical calculations with stable schemes and sufficiently fine meshes. We will not discuss the numerical approximation procedure in this paper, since that part is covered in numerous previous publications. The remaining part of the paper is organised as follows: In Section 2 we reiterate and complement the main findings in [59–64] and outline the general procedure for obtaining energy bounds in terms of external data. The error analysis is given in Section 3. A summary is provided in Section 4.

2. The governing initial boundary value problem

We start by recapitulating the results in [62–64]. Consider the following general hyperbolic IBVP

$$PU_t + (A_i(\bar{U})U)_{x_i} + A_i^T(\bar{U})U_{x_i} = F(\bar{x}, t), \quad t \geq 0, \quad \bar{x} = (x_1, x_2, ..., x_k) \in \Omega \quad (2.1)$$

augmented with the initial condition $U(\bar{x}, 0) = H(\bar{x})$ in $\Omega$ and the non-homogeneous boundary condition

$$L(\bar{U})U = G(\bar{x}, t), \quad t \geq 0, \quad \bar{x} = (x_1, x_2, ..., x_k) \in \partial \Omega. \quad (2.2)$$

In (2.1) and in the rest of the paper, Einstein’s summation convention with summation over repeated index is used. The time-independent matrix $P$ is symmetric positive definite and defines a scalar product $(U, V)_p = \int_\Omega U^T PV d\Omega$ and an energy norm $\|U\|_p^2 = (U, U)_p$. We further require that the eigenvalues of $P$ (and hence also of $P^{-1}$) are of order one. In (2.2), $F$ is a forcing function, $L$ is the boundary operator and $G$ the boundary data. $F$, $G$ and $H$ are the external input data. We assume that both $U$ and $\bar{U}$ are smooth. The $n \times n$ matrices $A_i$ are smooth functions of the $n$ component vector $\bar{U}$, but otherwise arbitrary. Note that (2.1) and (2.2) encapsulate both linear ($\bar{U} \neq U$) and nonlinear ($\bar{U} = U$) problems.

In [63,64] it was proved that the skew-symmetric form of (2.1) with boundary conditions such that

$$\int_{\partial \Omega} U^T(n_iA_i)U d\sigma = \int_{\partial \Omega} \frac{1}{2}U^T((n_iA_i) + (n_iA_i)^T)U d\sigma \geq -\int_{\partial \Omega} G^T G d\sigma \quad (2.3)$$

lead to energy conservation and an energy bound in terms of the data $F$, $G$ and $H$.

2.1. Modelling the effect of disturbed data

Consider the nonlinear problem (2.1) with solution $U$ and slightly disturbed data $F + \delta F$, $G + \delta G$ and $H + \delta H$. By subtracting the non-disturbed problem with solution $V$ from the disturbed one and linearising (see [62]) we find the evolution problem for the difference $W = U - V$ to be

$$PW_t + (A_i(U)W)_{x_i} + A_i^T(U)W_{x_i} = \delta F(\bar{x}, t), \quad t > 0, \quad \bar{x} = (x_1, x_2, ..., x_k) \in \Omega \quad (2.4)$$

$$L(U)W = \delta G(\bar{x}, t), \quad t > 0, \quad \bar{x} = (x_1, x_2, ..., x_k) \in \partial \Omega$$

$$W = \delta H(\bar{x}), \quad t = 0, \quad \bar{x} = (x_1, x_2, ..., x_k) \in \partial \Omega.$$

By the development in [63,64] we know that $U$ in (2.4) is bounded by data with an appropriate boundary operator $L(U)$. We will investigate the influence of the disturbed data $\delta F$, $\delta G$ and $\delta H$ on the deviation $W$ in (2.4) by assuming that only one of the error
sources are non-zero at a time, which enable us to assess their relative influence. The three types of errors in (2.4) are: $\delta F$ which represent errors in the forcing function, $\delta G$ which represent errors in boundary data, and finally $\delta H$ which represent errors in initial data.

2.2. Well posed dissipative boundary conditions

Next, we recapitulate the crucial role of the boundary operator originally studied in [59–61]. The energy method applied to (2.4) yields

$$\frac{1}{2} \frac{d}{dt} \| W \|_p^2 + \oint_{\partial \Omega} W^T (n_i A_i) W \, ds = \int_{\Omega} W^T \delta F \, d\Omega = (W, \delta F)_I,$$

(2.5)

where $(n_1, \ldots, n_k)^T$ is the outward pointing unit normal and $I$ is the identity matrix. In (2.5), only the symmetric part of $n_i A_i$ remains. Next we rotate the boundary term into the form

$$\oint_{\partial \Omega} W^T (n_i A_i) W \, ds = \oint_{\partial \Omega} C^T \Lambda \, C \, ds = \oint_{\partial \Omega} (C^+)^T \Lambda^+ \, C^+ + (C^-)^T \Lambda^- \, C^- \, ds,$$

(2.6)

where $R^T (n_i A_i) R = \Lambda = \text{diag}(\lambda_i)$, $C = R^{-1} W$. In (2.6), $\Lambda^+$ and $\Lambda^-$ denote the positive and negative parts of the real matrix $\Lambda = \text{diag}(\lambda_i)$ respectively, while $C^+$ and $C^-$ denote the corresponding rotated (or characteristic) variables. We will use a well posed dissipative boundary condition [64] of the form

$$\sqrt{|\Lambda^-|} C^- = \delta G.$$

(2.7)

**Remark 2.1.** For linear problems, the number of boundary conditions is equal to the number of $\lambda_i$ with the wrong sign [19,65], if the rotation matrix $R$ is non-singular. In the nonlinear case, it is more complicated since multiple forms of the boundary terms may exist since then $\Lambda = \Lambda(C)$ [30,62–64].

3. Error estimates due to the uncertainty in external data

Cauchy-Schwarz inequality and differentiating the norm leads to the following useful relations

$$\langle W, \delta F \rangle_I \leq \| W \|_p \| \delta F \|_{p^{-1}} \text{ and } \frac{1}{2} \frac{d}{dt} \| W \|_p^2 = \| W \|_p \frac{d}{dt} \| W \|_p.$$

(3.1)

Following [59–61], we next relate the outflow boundary terms to the $L_2$ norm of the solution as

$$\oint_{\partial \Omega} W^T P \, d\Omega \leq \| W \|^2_p \| P \|^2_p \leq \| W \|^2_p \| W \|^2_p \| P \|^2_p \leq \frac{\eta(t)}{\Xi} = \eta(t).$$

(3.2)

The relation $\eta(t)$ was shown in [59,61] to lead to an integrating factor $\exp(\theta(\xi, t))$ in (2.5) where

$$\theta(\xi, t) = \int_{\xi}^{t} \eta(\tau) d\tau \geq 0 \text{ with } \delta_0 > 0.$$

(3.3)

The function $\theta(\xi, t)$ is monotonically increasing in time since $\frac{\partial}{\partial t} (C^+)^T \Lambda^+ C^+ ds$, does not vanish for all time.

**Remark 3.1.** Adding dissipation in (2.1) would increase the magnitude of $\delta(t)$ and hence $\exp(\theta(\xi, t))$ [64].

3.1. Three different error estimates

Firstly we estimate the error or deviation for the case where $\delta F \neq 0, \delta G = 0, \delta H = 0$. The relation (2.5) augmented with the homogeneous version of (2.7), the relation (3.1) and (3.2) leads to

$$\frac{d}{dt} \| W \|_p + \eta(t) \| W \|_p \leq \| \delta F \|_{p^{-1}}.$$

(3.4)

The use of the integrating factor technique and the estimate (3.3) leads to

$$\| W \|_p \leq \int_{0}^{t} e^{-\theta(\tau)} \| \delta F \|_{p^{-1}} d\tau \leq \int_{0}^{t} e^{-\delta_0(t-\tau)} d\tau \| \delta F \|_{p^{-1}} \| \delta F \|_{p^{-1}} \| \delta F \|_{p^{-1}} \leq \frac{1}{\delta_0} (\| \delta F \|_{p^{-1}} \| \delta F \|_{p^{-1}} \| \delta F \|_{p^{-1}}).$$

(3.5)

Secondly we estimate the error or deviation for the case where $\delta F = 0, \delta G \neq 0, \delta H = 0$. The relation (2.6) augmented with the non-homogeneous version of (2.7) and the relation (3.2) leads to
\[
\frac{d}{dt} \|W\|_p^2 + 2\eta(t)\|W\|_p^2 = -2 \int_{\partial\Omega} (C^{-1})^T \Lambda^- C^{-1} \delta s = 2 \int_{\partial\Omega} (\delta G)^T \delta G ds = 2\|\delta G\|^2_{\partial\Omega}.
\] (3.6)

The use of the integrating factor technique and estimate (3.3) leads in this case to

\[
\|W\|_p^2 \leq 2 \int_0^t e^{-\delta_0(t-\tau)}\|\delta G\|^2_{\partial\Omega} d\tau \leq 2 \int_0^t e^{-2\delta_0(t-\tau)} d\tau (\|\delta G\|^2_{\partial\Omega})_{\text{max}} \leq \frac{1}{\delta_0} (\|\delta G\|^2_{\partial\Omega})_{\text{max}}.
\] (3.7)

Thirdly we estimate the error or deviation for the case where \(\delta F = 0, \delta G = 0, \delta H \neq 0\). The relation (2.6) augmented with the homogeneous version of (2.7) and the relation (3.2) leads to

\[
\frac{d}{dt} \|W\|_p^2 + 2\eta(t)\|W\|_p^2 = 0.
\] (3.8)

The use of the integrating factor technique and estimate (3.3) leads in this case directly to

\[
\|W\|_p^2 \leq e^{-2\delta_0(0,t)}\|\delta H\|_p^2 \leq e^{-2\delta_0(0,t)}\|\delta H\|_p^2.
\] (3.9)

3.2. **Effects on short and long time calculations**

For long times, the estimates (3.5), (3.7), (3.9) imply that the errors in initial data decay exponentially while the errors stemming from the forcing function and boundary data continue to grow. The ones from the forcing function grow faster than the errors due to boundary data. For short times, the estimates (3.5), (3.7), (3.9) lead respectively to the leading order approximations

\[
\|W\|_p \propto t\|\delta F\|_{p-1}\|_{\partial\Omega}^{\max}, \quad \|W\|_p \propto \sqrt{t}\|\delta G\|_{\partial\Omega}^{\max}, \quad \|W\|_p \propto \|\delta H\|_p.
\] (3.10)

The estimates (3.10) imply that errors in initial data dominate for small times.

The estimates (3.5), (3.7), (3.9) for long times together with the short time estimate (3.10) provide a qualitative description of the error development due to uncertain data, and what to focus on for error reduction. More quantitative information can possibly be obtained in specific cases where more detailed information about the error levels \(\delta F, \delta G, \delta H\) is known using UQ techniques.

4. **Summary**

We have investigated the influence of uncertain data on solutions to initial boundary value problems. Uncertainty in the forcing function, initial data and boundary data have been considered and their relative influence for short and long time calculations have been assessed. For short time calculations, uncertainty in the initial data dominate. As time grows, the influence of initial data vanishes exponentially fast. For long time calculations, the uncertainty in the forcing function and boundary data dominate. Errors due to the forcing function grow faster (linearly in time) than the ones due to the boundary data (which grows as the square root of time). The results indicate that for short time calculations, the initial conditions are important, but for long time calculations, focus should be on the forcing function and boundary conditions. Our qualitative results have impact on calculations where similar mathematical and numerical techniques are used for both short and long times, and can guide more quantitative specific investigations.

**CRediT authorship contribution statement**

**Jan Nordström:** Writing – review & editing, Writing – original draft, Validation, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization.

**Declaration of competing interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

**Data availability**

No data was used for the research described in the article.

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References


