Second order error bounds for POD-ROM methods based on first order divided differences

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A R T I C L E   I N F O

A B S T R A C T

This note proves for the heat equation that using BDF2 as time stepping scheme in POD-ROM methods with snapshots based on difference quotients gives both the optimal second order error bound in time and pointwise estimates.

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1. Introduction

Most numerical methods using reduced order models based on proper orthogonal decomposition (POD-ROM methods) apply basis functions based on the snapshots (or values at different times) of the full order model (FOM). Recently, it has been shown that adding their first divided differences to the snapshots, or even using only these divided differences to obtain the basis functions, allows for pointwise-in-time error bounds [1–4]. However, all pointwise-in-time error bounds in the literature are only first order with respect to time.

Although the first divided differences are only first order approximations to the time derivatives of the snapshots, we show in this note that for POD-ROM methods based only on them it is possible to obtain pointwise-in-time second order error bounds if the two step backward differentiation formula (BDF2) is used to integrate the POD-ROM equations. This result is a theoretical support for the observation that second

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order methods allow for larger step sizes than first order ones without spoiling the error, thus resulting in more efficient POD-ROM simulations.

2. Model problem and proper orthogonal decomposition

Throughout this note, standard notations for Sobolev spaces and their norms will be used. As a model problem, we consider the heat equation

$$
\begin{array}{rll}
\partial_t u(t, \mathbf{x}) - \nu \Delta u(t, \mathbf{x}) & = & f(t, \mathbf{x}), \quad (t, \mathbf{x}) \in (0, T] \times \Omega, \\
u(t, \mathbf{x}) & = & 0, \qquad (t, \mathbf{x}) \in (0, T] \times \partial\Omega, \\
u(0, \mathbf{x}) & = & u^0(\mathbf{x}), \quad \mathbf{x} \in \Omega,
\end{array}
$$

in a bounded domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$. Let C_p be the constant in the Poincaré inequality

$$
\|v\|_0 \le C_p \|\nabla v\|_0, \quad v \in H_0^1(\Omega). \tag{1}
$$

Let us denote by X_h^l a finite element space based on piece-wise continuous polynomials of degree l that satisfies the homogeneous Dirichlet boundary conditions. The semi-discrete Galerkin approximation, the FOM, consists in finding $u_h : [0, T] \to X_h^l$ such that

$$
(\partial_t u_h, v_h) + \nu(\nabla u_h, \nabla v_h) = (f, v_h), \quad \forall\, v_h \in X_h^l.
$$

If $u \in L^\infty(0, T; H^{l+1}(\Omega))$ and $\partial_t u \in L^2(0, T; H^{l+1}(\Omega))$, the following error estimation is well-known (see e.g., [5, Theorem 1.2]):

$$
\max_{0 \le s \le T} \left(\|(u - u_h)(s)\|_0 + h\|(u - u_h)(s)\|_1 \right) \le C(u) h^{l+1}. \tag{2}
$$

Fix $T > 0$ and set $\Delta t = T/M$. Let $t^n = n\Delta t$, $n = 0, \dots, M$, $N = M + 1$, and define the space

$$
\boldsymbol{U} = \mathrm{span}\left\{ \sqrt{N} w_0, \tau \frac{u_h(t^1) - u_h(t^0)}{\Delta t}, \tau \frac{u_h(t^2) - u_h(t^1)}{\Delta t}, \dots, \tau \frac{u_h(t^M) - u_h(t^{M-1})}{\Delta t} \right\},
$$

where w_0 is either $w_0 = u_h(t^0)$ or $w_0 = \bar{u}_h = \sum_{j=0}^{M} u_h(t^j)/(M+1)$, and τ is a time scale to make the snapshots dimensionally correct. The following analysis only requires $\tau > 0$. Denote $\boldsymbol{U} = \mathrm{span}\{y_h^1, y_h^2, \dots, y_h^N\}$. Let X be either $X = L^2(\Omega)$ or $X = H_0^1(\Omega)$, and denote the correlation matrix by $K = ((k_{i,j})) \in \mathbb{R}^{N \times N}$ with $k_{i,j} = (y_h^i, y_h^j)_X/N$, $i, j = 1, \dots, N$, and $(\cdot, \cdot)_X$ being the inner product in X. We denote by $\lambda_1 \ge \lambda_2 \dots \ge \lambda_d > 0$ the positive eigenvalues of K and by $\boldsymbol{v}_1, \dots, \boldsymbol{v}_d \in \mathbb{R}^N$ the associated eigenvectors. There are eigenvalues with $\mathcal{O}(\tau^2)$ when $\tau \to \infty$, and, when $\tau \to 0$, $\lambda_1 \to \|w_0\|_X^2$, while the other eigenvalues tend to 0. Thus, $\tau = \mathcal{O}(1)$ is an appropriate choice in practice. The orthonormal POD basis functions of $\boldsymbol{U}$ are given by $\varphi_k = (\sum_{j=1}^{N} v_k^j y_h^j)/(\sqrt{N}\sqrt{\lambda_k})$, where v_k^j is the jth component of $\boldsymbol{v}_k$. For any $1 \le r \le d$ denote by $\boldsymbol{U}^r = \mathrm{span}\{\varphi_1, \varphi_2, \dots, \varphi_r\}$, and denote by $P^r : X_h^l \to \boldsymbol{U}^r$ the X-orthogonal projection onto $\boldsymbol{U}^r$. Then, it holds

$$
\frac{1}{N} \sum_{j=1}^{N} \|y_h^j - P^r y_h^j\|_X^2 = \sum_{k=r+1}^{d} \lambda_k. \tag{3}
$$

The stiffness matrix of the POD basis is given by $S = ((s_{i,j})) \in \mathbb{R}^{d \times d}$, with $s_{i,j} = (\nabla \varphi_i, \nabla \varphi_j)_X$. If $X = L^2(\Omega)$ the following inequality holds for all $v \in \boldsymbol{U}$, see [6, Lemma 2],

$$
\|\nabla v\|_0 \le \sqrt{\|S\|_2} \|v\|_0. \tag{4}
$$

3. Error analysis

Let us denote by $D^1 v^n = (v^n - v^{n-1})/\Delta t$ and by $D^2 v^n = ((3/2)v^n - 2v^{n-1} + (1/2)v^{n-2})/\Delta t$, then the POD-ROM method is defined in the following way: Find $u_r^n \in \boldsymbol{U}^r$ such that

$$(Du_r^n, v) + \nu(\nabla u_r^n, \nabla v) = (f^n, v), \quad \forall\, v \in \boldsymbol{U}^r,$$

where $D = D^1$ for $n = 1$ and $D = D^2$ for $2 \leq n \leq M$.

Lemma 1. *Let $T > 0$, let X be a Banach space, $z^n = z(t^n) \in X$, then*

$$\max_{0 \leq k \leq M} \|z^k\|_X^2 \leq 2\|z^0\|_X^2 + \frac{2T^2}{M} \sum_{n=1}^{M} \left\|D^1 z_n\right\|_X^2, \tag{5}$$

$$\max_{0 \leq k \leq M} \|z^k\|_X^2 \leq 2\|\bar{z}\|_X^2 + \frac{8T^2}{M} \sum_{n=1}^{M} \left\|D^1 z_n\right\|_X^2, \quad with \quad \bar{z} = \sum_{j=0}^{M} z^j/(M+1). \tag{6}$$

Proof. The proof of (5) can be found in [1, Lemma 3.3]. For proving (6), we observe that

$$z^k = z^0 + \Delta t \sum_{n=1}^{k} D^1 z^n, \quad \bar{z} = z^0 + \frac{1}{M+1}\left(\Delta t D^1 z^1 + \cdots + \Delta t \sum_{n=1}^{M} D^1 z^n\right). \tag{7}$$

Taking norms yields $\|z^k\|_X \leq \|z^0\|_X + \Delta t \sum_{n=1}^{M} \left\|D^1 z^n\right\|_X$ and $\|z^0\|_X \leq \|\bar{z}\|_X + \Delta t \sum_{n=1}^{M} \left\|D^1 z^n\right\|_X$, so that

$$\|z^k\|_X \leq \|\bar{z}\|_X + 2\Delta t \sum_{n=1}^{M} \left\|D^1 z^n\right\|_X \leq \|\bar{z}\|_X + 2T^{1/2}(\Delta t)^{1/2}\left(\sum_{n=1}^{M} \left\|D^1 z^n\right\|_X^2\right)^{1/2},$$

from which we reach (6). $\square$

In the sequel we define $\tilde{C} = 1$ if $w_0 = u_h(t^0)$ and $\tilde{C} = 4$ if $w_0 = \bar{u}_h$, and $C_X = 1$ if $X = L^2(\Omega)$ and $C_X = C_p^2$ f $X = H_0^1(\Omega)$.

Lemma 2. *The following bound holds*

$$\max_{0 \leq n \leq M} \|u_h^n - P^r u_h^n\|_0^2 \leq \left(2 + 4\tilde{C}\frac{T^2}{\tau^2}\right) C_X \sum_{k=r+1}^{d} \lambda_k. \tag{8}$$

Proof. Taking $z = u_h - P^r u_h$ in (5) or (6), depending on the selection of the first element in $\boldsymbol{U}$, and applying (3) and $N \leq 2M$, we reach (8). $\square$

Lemma 3. *Let $\{z^n\}_{n=0}^N \in \boldsymbol{U}^r$ and $\{\tau_1^n\}_{n=1}^N, \{\tau_2^n\}_{n=1}^N \in X_h^l$ satisfying*

$$(Dz^n, v) + \nu(\nabla z^n, \nabla v) = (\tau_1^n, v) + \nu(\nabla \tau_2^n, \nabla v), \quad \forall\, v \in \boldsymbol{U}^r, \tag{9}$$

where $D = D^1$ for $n = 1$ and $D = D^2$ for $2 \leq n \leq M$. Then, it holds for $\Delta t < T/4$ and $n \geq 1$

$$\|z^n\|_0^2 + 2\nu \sum_{j=1}^{n} \Delta t\|\nabla z^j\|_0^2 \leq e^4 \left(17\|z^0\|_0^2 + 28(\Delta t)^2 \left\|\tau_1^1\right\|_0^2 + 2\Delta t T \sum_{j=2}^{N} \|\tau_1^n\|_0^2 \right.$$

$$\left. + 14\nu \Delta t\|\nabla \tau_2^1\|_0^2 + 2\nu \Delta t \sum_{j=2}^{N} \|\nabla \tau_2^n\|_0^2\right). \tag{10}$$

Proof. We take $v = \Delta t z^n$ in (9). If $n = 1$ then $D = D^1$ and Young's inequality yields

$$\frac{1}{2}\|z^1\|_0^2 - \frac{1}{2}\|z^0\|_0^2 + \nu\Delta t\|\nabla z^1\|_0^2 \leq \Delta t(\tau_1^1, z^1) + \nu\Delta t(\nabla\tau_2^1, \nabla z^1). \tag{11}$$

For $n \geq 2$ then $D = D^2$ and one gets

$$\frac{1}{4}\|z^n\|_0^2 + \frac{1}{4}\|\hat{z}^n\|_0^2 - \frac{1}{4}\|z^{n-1}\|_0^2 - \frac{1}{4}\|\hat{z}^{n-1}\|_0^2 + \nu\Delta t\|\nabla z^n\|_0^2 \leq \Delta t(\tau_1^n, z^n) + \nu\Delta t(\nabla\tau_2^n, \nabla z^n),$$

where $\hat{z}^n = 2z^n - z^{n-1}$. The Cauchy–Schwarz and Young inequality give

$$\Delta t(\tau_1^n, z^n) + \nu\Delta t(\nabla\tau_2^n, \nabla z^n) \leq \frac{\Delta t}{2T}\|z^n\|_0^2 + \frac{T\Delta t}{2}\|\tau_1^n\|_0^2 + \Delta t\frac{\nu}{2}\|\nabla z^n\|_0^2 + \Delta t\frac{\nu}{2}\|\nabla\tau_2^n\|_0^2. \tag{12}$$

Multiplying by 4, applying (12), and summing from 2 to n, one gets

$$\|z^n\|_0^2 + 2\nu\sum_{j=2}^{n}\Delta t\|\nabla z^j\|_0^2 \leq \|z^1\|_0^2 + \|\hat{z}^1\|_0^2 + 2\sum_{j=2}^{n}\frac{\Delta t}{T}\|z^j\|_0^2 + 2T\sum_{j=2}^{n}\Delta t\|\tau_1^j\|_0^2 + 2\nu\sum_{j=2}^{n}\Delta t\|\nabla\tau_2^j\|_0^2. \tag{13}$$

Young's inequality yields $\|\hat{z}^1\|_0^2 \leq 6\|z^1\|_0^2 + 3\|z^0\|^2$, so that $\|z^1\|_0^2 + \|\hat{z}^1\|_0^2 \leq 7\|z^1\|_0^2 + 3\|z^0\|^2$. Using again Young's inequality gives

$$\Delta t(\tau_1^1, z^1) + \nu\Delta t(\nabla\tau_2^1, \nabla z^1) \leq \frac{1}{4}\left\|z^1\right\|_0^2 + (\Delta t)^2\left\|\tau_1^1\right\|_0^2 + \Delta t\frac{\nu}{2}\left\|\nabla z^1\right\|_0^2 + \Delta t\frac{\nu}{2}\left\|\nabla\tau_2^1\right\|_0^2,$$

so that we obtain from (11)

$$\left\|z^1\right\|_0^2 + 2\nu\Delta t\left\|\nabla z^1\right\|_0^2 \leq 2\left\|z^0\right\|_0^2 + 4(\Delta t)^2\left\|\tau_1^1\right\|_0^2 + 2\Delta t\nu\left\|\nabla\tau_2^1\right\|_0^2.$$

Together with (13), it follows that for $n \geq 1$

$$\|z^n\|_0^2 + 2\nu\sum_{j=1}^{n}\Delta t\|\nabla z^j\|_0^2 \leq 17\|z^0\|_0^2 + 28(\Delta t)^2\left\|\tau_1^1\right\|_0^2 + 2\sum_{j=2}^{n}\frac{\Delta t}{T}\|z^j\|_0^2 + 2T\sum_{j=2}^{n}\Delta t\|\tau_1^j\|_0^2$$

$$+ 14\Delta t\nu\|\nabla\tau_2^1\|_0^2 + 2\nu\sum_{j=1}^{n}\Delta t\|\nabla\tau_2^j\|_0^2,$$

from where (10) follows by applying Gronwall's Lemma [7, Lemma 5.1] for $\Delta t \leq T/4$. $\quad\square$

Let $X = L^2(\Omega)$ and let us denote by $e_r^n = u_r^n - P^r u_h^n$ and by $\eta_h^n = P^r u_h^n - u_h^n$. Arguing as in the proof of [2, Theorem 4.6], one gets

$$(De_r^n, v) + \nu(\nabla e_r^n, \nabla v) = (\partial_t u_h^n - Du_h^n, v) - \nu(\nabla\eta_h^n, \nabla v), \quad \forall\, v \in \boldsymbol{U}^r. \tag{14}$$

Lemma 4. *The following bounds hold*

$$\left\|\partial_t u_h^1 - D^1 u_h^1\right\|_j \leq \frac{\Delta t}{2}\max_{0\leq t\leq t_1}\|\partial_{tt}u_h\|_j, \quad j = 0, 1, \tag{15}$$

$$\left\|\partial_t u_h^n - D^2 u_h^n\right\|_j \leq \sqrt{5}(\Delta t)^{3/2}\left(\int_{t_{n-2}}^{t_n}\|\partial_{ttt}u_h(t)\|_j^2\,dt\right)^{1/2}, \quad n = 2,\ldots,N, \; j = 0, 1. \tag{16}$$

Proof. For $D = D^1$, (15) follows easily from

$$\partial_t u_h^n - Du_h^n = \frac{1}{\Delta t}\int_{t_{n-1}}^{t_n}(\partial_t u_h(t_n) - \partial_t u_h(s))\,ds = \frac{1}{\Delta t}\int_{t_{n-1}}^{t_n}\left(\int_s^{t_n}\partial_{tt}u_h(t)\,dt\right)ds.$$

For $D = D^2$, Taylor series expansion with integral reminder reveals that

$$\partial_t u_h^n - D u_h^n = \frac{1}{\Delta t} \int_{t_{n-2}}^{t_n} \left(2(t - t_{n-1})_+^2 - \frac{1}{2}(t - t_{n-2})^2 \right) \partial_{ttt} u_h \, dt,$$

where $x_+ = \max(0, x)$, for $x \in \mathbb{R}$. Then, a straightforward calculation shows that

$$\| \partial_t u_h^n - D u_h^n \|_j \leq \left(\frac{2}{\sqrt{5}} + \frac{2\sqrt{2}}{\sqrt{5}} \right) (\Delta t)^{3/2} \left(\int_{t_{n-2}}^{t_n} \| \partial_{ttt} u_h(t) \|_j^2 \, dt \right)^{1/2},$$

and then (16) follows by noticing that $2 + 2\sqrt{2} < 5$. $\quad\square$

Lemma 5. *Let $X = L^2(\Omega)$. It holds*

$$\nu \sum_{j=1}^n \Delta t \| \nabla \eta_h^j \|_0^2 \leq \nu T \| S \|_2 \left(2 + 4\tilde{C} \frac{T^2}{\tau^2} \right) \sum_{k=r+1}^d \lambda_k. \tag{17}$$

Proof. The proof of (17) follows easily by applying (4) and (8). $\quad\square$

Theorem 1 (*Bound for $X = L^2(\Omega)$*). *Let $X = L^2(\Omega)$, then it holds for $\Delta t \leq T/4$*

$$\max_{1 \leq n \leq M} \| u_r^n - u^n \|_0^2 \leq 60 e^4 \left(\| e_r^0 \|_0^2 + (\Delta t)^4 \max_{0 \leq s \leq \Delta t} \| \partial_{tt} u_h(s) \|_0^2 + T(\Delta t)^4 \int_0^T \| \partial_{ttt} u_h(s) \|_0^2 \, ds \right)$$

$$+ 3(1 + 14T\nu e^4 \| S \|_2) \left(2 + 4\tilde{C} \frac{T^2}{\tau^2} \right) \sum_{k=r+1}^d \lambda_k + 3C(u)^2 h^{2(l+1)}. \tag{18}$$

Proof. From (10) and (14), applying (15), (16) (noting that most integrals over time intervals $[t_{j-1}, t_j]$ appear twice when summing over n), and (17), we obtain

$$\| e_r^n \|_0^2 + \nu \sum_{j=1}^n \Delta t \| \nabla e_r^j \|_0^2 \leq e^4 \left(17 \| e_r^0 \|_0^2 + 7(\Delta t)^4 \max_{0 \leq s \leq \Delta t} \| \partial_{tt} u_h(s) \|_0^2 \right.$$

$$\left. + 20T(\Delta t)^4 \int_0^T \| \partial_{ttt} u_h(s) \|_0^2 ds + 14\nu T \| S \|_2 \left(2 + 4\tilde{C} \frac{T^2}{\tau^2} \right) \sum_{k=r+1}^d \lambda_k \right).$$

To simplify, we replace the factors 17 and 7 and 20 by their maximum. To finish the proof, apply the decomposition $u_r^n - u^n = (u_r^n - P_h u_h^n) + (P_h u_h^n - u_h^n) + (u_h^n - u^n)$, followed by (2) and (8). $\quad\square$

Let $X = H_0^1(\Omega)$. Arguing as in the proof of [2, Theorem 4.1] yields

$$(De_r^n, v) + \nu(\nabla e_r^n, \nabla v) = (\partial_t u_h^n - P_r (D u_h^n), v), \quad \forall v \in \boldsymbol{U}^r.$$

Applying Lemma 3 with $z^n = e_r^n$, $\tau_1^n = \partial_t u_h^n - P_r D u_h^n$ and $\tau_2 = 0$ we get

$$\| e_r^n \|_0^2 + 2\nu \sum_{j=1}^n \Delta t \| \nabla e_r^j \|_0^2 \leq e^4 \left(17 \| e_r^0 \|_0^2 + 28(\Delta t)^2 \left\| \tau_1^1 \right\|_0^2 + 2\Delta t T \sum_{j=2}^N \| \tau_1^n \|_0^2 \right). \tag{19}$$

Theorem 2 (*Bound for $X = H_0^1(\Omega)$*). *Let $X = H_0^1(\Omega)$, $\Delta t \leq T/4$, and $C_1 = 4e^4 (10 + \Delta t/T) + 2 + 4\tilde{C}$. Then it holds*

$$\max_{1 \leq n \leq M} \|u_r^n - u^n\|_0^2 \leq 60e^4 \left(\|e_r^0\|_0^2 + (\Delta t)^4 \max_{0 \leq s \leq \Delta t} \|\partial_{tt} u_h(s)\|_0^2 + 2(\Delta t)^4 \int_0^T \|\partial_{ttt} u_h(t)\|_0^2 \, dt \right)$$

$$+ 3C_1 C_p^2 \left(\frac{T}{\tau} \right)^2 \sum_{j=r+1}^d \lambda_k + 3C^2(u) h^{2(l+1)}. \tag{20}$$

Proof. The last two terms on the right-hand side of (19) are bounded by the triangle inequality

$$\|\tau_1^n\|_0^2 = \|\partial_t u_h^n - P^r (Du_h^n)\|_0^2 \leq 2 \|\partial_t u_h^n - (Du_h^n)\|_0^2 + 2 \|(I - P^r)(Du_h^n)\|_0^2. \tag{21}$$

For $n = 1$, the first term is bounded by (15) and the second one by (1) and (3), giving

$$(\Delta t)^2 \left\|\tau_1^1\right\|_0^2 \leq \frac{(\Delta t)^4}{2} \max_{0 \leq s \leq \Delta t} \|\partial_{tt} u_h(s)\|_0^2 + \frac{4T}{\tau^2} C_p^2 \Delta t \sum_{k=r+1}^d \lambda_k.$$

For $n \geq 2$, the first term of (21) is estimated by (16). To bound the other term observe that

$$D^2 u_h^n = \frac{3}{2} D^1 u^n - \frac{1}{2} D^1 u^{n-1},$$

and, consequently,

$$2 \left\|(I - P^r)(D^2 u_h^n)\right\|_0^2 \leq \frac{9}{2} \left\|(I - P^r)(D^1 u_h^n)\right\|_0^2 + \frac{1}{2} \left\|(I - P^r)(D^1 u_h^n)\right\|_0^2,$$

so that, by using (1) and (3), one obtains

$$2T \sum_{j=2}^n \Delta t \left\|(I - P^r)(D^2 u_h^n)\right\|_0^2 \leq 10T \sum_{j=1}^n \Delta t \left\|(I - P^r)(D^1 u_h^n)\right\|_0^2 \leq 20 C_p^2 \left(\frac{T}{\tau} \right)^2 \sum_{j=r+1}^d \lambda_k.$$

Collecting the estimates for $n = 1$ and $n \geq 2$ leads to

$$\|e_r^n\|_0^2 + 2\nu \sum_{j=1}^n \Delta t \|\nabla e_r^j\|_0^2 \leq e^4 \left(17\|e_r^0\|_0^2 + 14(\Delta t)^4 \max_{0 \leq s \leq \Delta t} \|\partial_{tt} u_h(s)\|_0^2 \right.$$

$$\left. + 40(\Delta t)^4 \int_0^T \|\partial_{ttt} u_h(t)\|_0^2 \, dt + 4 \left(10 + \frac{\Delta t}{T} \right) C_p^2 \frac{T^2}{\tau^2} \sum_{j=r+1}^d \lambda_k \right).$$

Now, the proof is finished in the same way as the proof of Theorem 1. $\square$

Second order error bounds in time of form (18) and (20) can be derived if the finite differences in $\boldsymbol{U}$ are replaced with the temporal derivatives $\{\partial_t u_h^n\}_{n=0}^M$, with only slight modifications in the analysis. If the set of snapshots is $\{u_h^n\}_{n=0}^M$, then a second order estimate for $\sum_{j=1}^M \Delta t \|u_r^n - u^n\|_0^2$ can be shown along the lines of the presented analysis but neither pointwise estimates nor optimal estimates in the H^1 norm seem to be possible with the present approach, for the reasons explained in [3]. If for a problem an analysis for a first order temporal discretization is known, like for the incompressible Navier–Stokes equations in [2], it can be extended to BDF2 using the techniques of this note to handle the temporal discretization.

Data availability

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

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