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Equivalence between the DPG method and the exponential integrators for linear parabolic problems

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ABSTRACT

The Discontinuous Petrov-Galerkin (DPG) method and the exponential integrators are two well established numerical methods for solving Partial Differential Equations (PDEs) and stiff systems of Ordinary Differential Equations (ODEs), respectively. In this work, we apply the DPG method in the time variable for linear parabolic problems and we calculate the optimal test functions analytically. We show that the DPG method in time is equivalent to exponential integrators for the trace variables, which are decoupled from the interior variables. In addition, the DPG optimal test functions allow us to compute the approximated solutions in the time element interiors. This DPG method in time allows to construct a posteriori error estimations in order to perform adaptivity. We generalize this novel DPG-based time-marching scheme to general first order linear systems of ODEs. We show the performance of the proposed method for 1D and 2D + time linear parabolic PDEs after discretizing in space by the finite element method.

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1. Introduction

The Discontinuous Petrov-Galerkin (DPG) method with optimal test functions for approximating the solution of Partial Differential Equations (PDEs) was proposed by Demkowicz and Gopalakrishnan in 2010 [9,11]. Since then, it has been applied to a wide variety of problems including linear elasticity [5], Maxwell's equations [7], convection-dominated diffusion [8,16,17], Poisson equation [10], Stokes' flow [19] and Helmholtz equation [14,37], among many others. For more recent overviews, see [12,13,23]. The key idea of the DPG method is to construct optimal test functions in such a way that the discrete stability is inherited from the continuous method. Here, the optimal test functions realize the supremum of the discrete inf-sup condition guaranteeing the stability of the numerical method.

In this article, we focus on the DPG method in time. There exist previous works on DPG for time domain problems. In [18,20], authors apply the DPG method in both space and time variables at the same time for parabolic problems, in [15] for Schrödinger equation, and in [24] for the wave equation. The downside of this approach is that in 3D + time problems, 4D meshes are needed. In [22], authors introduce and analyze a numerical scheme for the heat equation where they apply the backward Euler method in time and DPG in space.

In contrast to previous works, in here we seek to apply the DPG method in time dimension in order to have a time-stepping scheme also coming from the DPG theory. The goal is to achieve an efficient and simple method that fits into the

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DPG methodology. One of the advantages of our approach is that optimal test functions are readily available in 1D. This is not the case in most DPG methods, where an approximation to the optimal test functions is calculated on the fly employing conforming discontinuous test functions from broken spaces.

In this work, we start from a single first order ODE and we derive a suitable ultraweak formulation in time. Then, we calculate the optimal test functions of the DPG method analytically, which leads to exponentials that depend upon the data of the problem. When we substitute the optimal test functions in the ultraweak formulation, we obtain a representation called "variation-of-constants formula" for the trace variables and those are completely decoupled from the system. Then, we generalize the proposed method to a general linear system of ODEs where the optimal test functions are exponentials of matrices. We prove that we can either: (a) apply the DPG method for a single interval and employ the resulting trace solution as an initial value for the next interval, or (b) formulate the optimal testing problem globally. Both approaches provide exactly the same solution. We show the performance of this method for single ODEs and linear parabolic problems (1D and 2D + time) after discretizing in space by the finite element method.

In both cases (a single ODE and a system of ODEs) we show that the resulting trace variables are calculated by the variation-of-constants formula, which is equivalent to the use of exponential integrators [27,29]. The latter are a class of methods for the integration in time of stiff systems of Ordinary Differential Equations (ODEs) that have many applications [3,26,32,35,36]. They are mostly employed to solve semilinear systems of the form $u'(t) = Lu(t) + f(u(t), t)$ where L is a linear operator and f is nonlinear. In this method, the exact solution of the system is expressed by the variation-of-constants formula. Different approximations of such a representation lead to different methods like exponential Runge-Kutta methods [28], Rosenbrock method [31], and exponential multistep methods [30], among many others. All of them involve the computation of the exponential of a matrix and related functions (called φ-functions). There exist an extensive literature on how to efficiently compute matrix exponentials and the φ-functions [1,4,6,33,34]. For a recent overview, see [25]. Here, we consider linear ODE systems (i.e. f does not depend on u) and for the numerical results, we employ the MATLAB package called EXPINT [4] that employs the scaling and squaring method defined in [33] and a Padé approximant to calculate the matrix exponentials.

Summarizing, we prove that the DPG method in time for parabolic problems is equivalent to exponential integrators for the trace variables. A unique feature of the DPG method is that it provides an approximation in the interiors of the elements given by the orthogonal projection of the exact solution into the discrete trial space. For computational purposes, we express the resulting DPG-based time-marching-scheme in terms of φ-functions because the computation of such functions of matrices is a well studied research topic and there is a wide range of software available [25]. Finally, since the resulting method is DPG, it is possible to analyze it from the variational point of view and apply adaptive strategies previously studied in the DPG community. Such technology is unavailable in the exponential integrators community and its development is left as future work.

This article is organized as follows. Section 2 states the strong and ultraweak formulations of a single linear ODE. Section 3 describes the ideal Petrov-Galerkin method and we provide the analytical solution of the optimal test functions for this case. In Section 4, we calculate the optimal test functions when we select a trial space composed of polynomials of order p. In Section 5, we present the ideal DPG method as a time-marching scheme. Section 6 generalizes the ideal DPG method for a linear system of ODEs. Section 7 explains the relation of the ideal DPG method with the exponential integrators on the trace variables and describes the approximation employed in the element interiors. Section 8 presents the numerical results for a single ODE, the 1D + time heat equation and the 2D + time Eriksson-Johnson problem. Section 9 summarizes the conclusions and possible extensions of this work. Finally, Appendix A provides the proofs of the theoretical results stated in this article.

2. Single Ordinary Differential Equation (ODE)

Let $I = (0, 1] \subset \mathbb{R}$, we consider the following first order Ordinary Differential Equation (ODE)

$$\begin{cases} u' + \lambda u = f & \text{in } I, \\ u(0) = u_0, \end{cases} \tag{1}$$

where $\lambda \in \mathbb{R}\backslash\{0\}$ and $f \in L^2(I)$. Here, the source term $f(t)$ and the initial condition $u_0 \in \mathbb{R}$ are given data.

To obtain a variational formulation of problem (1), we multiply the equation by some suitable test functions v and we integrate over I

$$\int_I (u' + \lambda u) v \, dt = \int_I f v \, dt,$$

and we integrate by parts

$$-\int_I u v' \, dt + u(1)v(1) - u(0)v(0) + \int_I \lambda u v \, dt = \int_I f v \, dt.$$

Now, we substitute $u(0)$ by u_0 in the last equation and we treat the unknown value $u(1)$ as another variable $\hat{u}$. We then obtain the following ultraweak variational formulation of problem (1)

$$\begin{cases} \text{Find } z = (u, \hat{u}) \in U \text{ such that} \\ \quad b(z, v) = l(v), \ \ \forall v \in V, \end{cases} \tag{2}$$

where the trial and test spaces are

$$U = U_0 \times \hat{U} = L^2(I) \times \mathbb{R}, \ \ V = H^1(I),$$

and we define

$$b(z, v) := -\int_I u v' \, dt + \int_I \lambda u v \, dt + \hat{u} v(1),$$
$$l(v) := \int_I f v \, dt + u_0 v(0).$$

Finally, we define the following norms in U and V

$$\begin{aligned} ||z||_U^2 &:= ||u||^2 + |\hat{u}|^2, \\ ||v||_V^2 &:= ||-v' + \lambda v||^2 + |v(1)|^2, \end{aligned} \tag{3}$$

where $||\cdot||$ denotes the usual norm in $L^2(I)$.

3. Petrov-Galerkin (PG) method with optimal test functions

3.1. Overview

Given a discrete subspace $U_h = U_{h,0} \times \hat{U} \subset U$ and $(\cdot,\cdot)_V$ an inner product in V with norm $||\cdot||_V$, we introduce the *trial-to-test operator* $\Phi : U_h \longrightarrow V$ defined by

$$(\Phi z_h, v)_V = b(z_h, v), \ \forall v \in V, \ z_h \in U_h, \tag{4}$$

and we define the *optimal test space* for the continuous bilinear form $b(\cdot,\cdot)$ as $V_h^{opt} := \Phi(U_h)$. Note that from (4), we have that $dim\ V_h^{opt} = dim\ U_h$. We now introduce the *ideal Petrov-Galerkin (PG) method* as

$$\begin{cases} \text{Find } z_h = (u_h, \hat{u}_h) \in U_h \text{ such that} \\ \quad b(z_h, v_h) = l(v_h), \ \ \forall v_h \in V_h^{opt}. \end{cases} \tag{5}$$

Theorem 1. *Suppose* $\{z \in U \mid b(z, v) = 0, \ \forall v \in V\} = \{0\}$ *and that there exist* $M, \gamma > 0$ *such that*

$$\gamma ||v||_V \leq \sup_{0 \neq z \in U} \frac{|b(z, v)|}{||z||_U} \leq M ||v||_V, \ \forall v \in V,$$

then the solution z_h *of the ideal PG method (5) is unique and it holds*

$$||z - z_h||_U \leq \frac{M}{\gamma} \inf_{w_h \in U_h} ||z - w_h||_U,$$

where z *is the exact solution of (2). It also holds that* z_h *is the best approximation to* z *in the energy norm defined by* $||z||_E := \sup_{0 \neq v \in V} \frac{|b(z, v)|}{||v||_V}$, *i.e.,*

$$||z - z_h||_E = \inf_{w_h \in U_h} ||z - w_h||_E.$$

Proof. See [12]. □

If we consider problem (2) with the variational setting defined in Section 2, Theorem 1 holds with $M = \gamma = 1$ with respect to the norms defined in (3) [23].

3.2. Optimal test functions

We now calculate the optimal test functions by solving (4) analytically. Given a trial function $z_h = (u_h, \hat{u}_h) \in U_h$, we find $v \in V$ such that

$$(v, \delta v)_V = b(z_h, \delta v), \quad \forall \delta v \in V, \tag{6}$$

which is equivalent to

$$\int_I (-v' + \lambda v)(-(\delta v)' + \lambda \delta v)dt + v(1)\delta v(1) = \int_I u_h(-(\delta v)' + \lambda \delta v)dt + \hat{u}_h \delta v(1). \tag{7}$$

Integrating by parts in time, we obtain

$$\int_I (-v'' + \lambda^2 v)\delta v dt + (v'(1) - \lambda v(1) + v(1))\delta v(1) + (-v'(0) + \lambda v(0))\delta v(0)$$
$$= \int_I (u_h' + \lambda u_h)\delta v dt + (\hat{u}_h - u_h(1))\delta v(1) + u_h(0)\delta v(0).$$

From Fourier's lemma, this is equivalent to the following Boundary Value Problem (BVP) governed by an ODE

$$\begin{cases} -v'' + \lambda^2 v = u_h' + \lambda u_h, \\ -v'(0) + \lambda v(0) = u_h(0), \\ v'(1) - \lambda v(1) + v(1) = -u_h(1) + \hat{u}_h, \end{cases} \tag{8}$$

whose solution is

$$\Phi(u_h, \hat{u}_h) = e^{\lambda(t-1)}\hat{u}_h + e^{\lambda t}\int_t^1 e^{-\lambda\tau} u_h(\tau)d\tau. \tag{9}$$

Remark 1. Note that solution (9) also satisfies the following BVP

$$\begin{cases} -v' + \lambda v = u_h, \\ v(1) = \hat{u}_h. \end{cases} \tag{10}$$

For the proof (10)$\Longleftrightarrow$(8), see Appendix A. This result comes from selecting the adjoint norm in problem (6). Therefore, the optimal test functions are solutions of the strong form of the adjoint equation. Moreover, this is equivalent to the idea of optimal test functions introduced by Barret and Morton in [2].

Remark 2. Authors in [9] proved that for the transport equation in 1D over a single element, if we select polynomials of order p for the discrete trial space U_h, then the optimal test space is composed of polynomials of order $p+1$. Our construction is, indeed, consistent with this result. Note that for $\lambda = 0$ in (1), we have the transport equation and the trial-to-test operator defined in (9) becomes

$$\Phi(u_h, \hat{u}_h) = \hat{u}_h + \int_t^1 u_h(\tau)d\tau.$$

Therefore, the optimal test functions are integrals of the trial functions.

Finally, if we solve problem (5) with the optimal test functions defined by the trial-to-test operator (9), we have that z_h is the orthogonal projection of the exact solution z into U_h with respect to the norm defined in (3).

4. Optimal test functions for polynomials of order p

We consider the discrete trial space $U_h = U_{h,0} \times \hat{U}$ where $U_{h,0}$ is composed of polynomials of order p. Then, we can express the solution $z_h = (u_h, \hat{u}_h) \in U_h$ of problem (5) as in Fig. 1, where

$$u_h = \sum_{j=0}^{p} u_{h,j} t^j.$$

We study the optimal test functions for U_h and the resulting schemes employing the trial-to-test operator defined in (9).

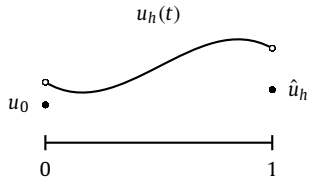


Fig. 1. Solution of problem (5).

4.1. Lowest order case ($p = 0$)

We select for $U_{h,0}$ the space of constant functions in time. We have

$$\hat{v}(\lambda, t) := \Phi(0, 1) = e^{\lambda(t-1)}, \quad v_0(\lambda, t) := \Phi(1, 0) = \frac{1 - e^{\lambda(t-1)}}{\lambda}, \tag{11}$$

so $V_h^{opt} = span\left\{\hat{v}, v_0\right\}$ and we have from Remark 1 that

$$\begin{cases} -\hat{v}'(\lambda, t) + \lambda\hat{v}(\lambda, t) = 0, & \hat{v}(\lambda, 1) = 1, \\ -v_0'(\lambda, t) + \lambda v_0(\lambda, t) = 1, & v_0(\lambda, 1) = 0, \end{cases}$$

where v_0' denotes the derivative of v_0 with respect to time. Then, solving problem (5), we obtain

$$\begin{cases} \hat{u}_h = u_0\hat{v}(\lambda, 0) + \displaystyle\int_0^1 f(t)\hat{v}(\lambda, t)dt, \\ u_{h,0} = u_0 v_0(\lambda, 0) + \displaystyle\int_0^1 f(t)v_0(\lambda, t)dt. \end{cases} \tag{12}$$

4.2. Polynomials of order p

We calculate $\Phi(t^p, 0)$ recursively as

$$\begin{aligned} v_p(\lambda, t) := \Phi(t^p, 0) &= e^{\lambda t}\int_t^1 e^{-\lambda\tau}\tau^p d\tau = e^{\lambda t}\left[\frac{\tau^p}{-\lambda}e^{-\lambda\tau}\right]_t^1 + \frac{p}{\lambda}e^{\lambda t}\int_t^1 e^{-\lambda\tau}\tau^{p-1}d\tau \\ &= \frac{t^p}{\lambda} - \frac{1}{\lambda}e^{\lambda(t-1)} + \frac{p}{\lambda}\Phi(t^{p-1}, 0). \end{aligned}$$

Equivalently

$$v_p(\lambda, t) = \frac{1}{\lambda}\left(t^p + p v_{p-1}(\lambda, t) - \hat{v}(\lambda, t)\right). \tag{13}$$

Here, $V_h^{opt} = span\{\hat{v}, v_r, \ \forall r = 0, \ldots, p\}$ and (13) can be expressed as (see Appendix A for details)

$$v_p(\lambda, t) = \frac{1}{\lambda^{p+1}}\left(\mathcal{P}_p(\lambda, t) - \mathcal{P}_p(\lambda, 1)\hat{v}(\lambda, t)\right), \tag{14}$$

where $\mathcal{P}_p(\lambda, t)$ is a polynomial of order p defined as

$$\mathcal{P}_p(\lambda, t) = \sum_{j=0}^{p}\frac{p!}{j!}(\lambda t)^j.$$

Directly from (10), as we select $u_h = t^p$, we have the following property

$$-v_p'(\lambda, t) + \lambda v_p(\lambda, t) = t^p. \tag{15}$$

Finally, as $v_p(\lambda, 1) = 0$, problem (5) becomes

$$\begin{cases} \hat{u}_h = u_0 \hat{v}(\lambda, 0) + \int_0^1 f(t)\hat{v}(\lambda, t)dt, \\ \int_0^1 \left(\sum_{j=0}^{p} u_{h,j} t^j \right) t^r dt = u_0 v_r(\lambda, 0) + \int_0^1 f(t) v_r(\lambda, t)dt, \ \ \forall r = 0, \ldots, p. \end{cases} \tag{16}$$

We will see in Section 7 that scheme (16) is equivalent to the so-called exponential integrator for the trace variables.

5. Ideal discontinuous Petrov-Galerkin (DPG) method

We now consider a partition I_h of the time interval I as

$$0 = t_0 < t_1 < \ldots < t_{m-1} < t_m = 1, \tag{17}$$

and we define $I_k = (t_{k-1}, t_k)$ and $h_k = t_k - t_{k-1}$, $\forall k = 1, \ldots, m$. We introduce the following broken test space

$$V = H^1(I_h) = \{v \in L^2(I) \mid v_{|_{I_k}} \in H^1(I_k), \ \forall I_k \in I_h\},$$

with associated norm

$$||v||_V^2 = \sum_{k=1}^{m} \int_{I_k} |-v' + \lambda v|^2 dt + [v]_k^2.$$

Here, we define $v(t_k^{\pm}) := \lim_{\varepsilon \to 0^+} v(t_k \pm \varepsilon)$, $[v]_k = v(t_k^+) - v(t_k^-)$, $\forall k = 1, \ldots, m-1$, and $[v]_m = -v(t_m^-)$. We set $U = U_0 \times \hat{U} = L^2(I) \times \mathbb{R}^m$, $z = (u, \hat{u}^1, \ldots, \hat{u}^m)$ and also

$$||z||_U^2 = ||u||^2 + \sum_{k=1}^{m} |\hat{u}^k|^2,$$

$$b(z, v) = \sum_{k=1}^{m} \int_{I_k} u(-v' + \lambda v)dt - \hat{u}^k [v]_k.$$

Given a discrete subspace $U_h = U_{h,0} \times \hat{U} \subset U$ and $(\cdot, \cdot)_V$ an inner product in V, the *ideal Discontinuous Petrov-Galerkin (DPG)* method reads

$$\begin{cases} \text{Find } z_h = (u_h, \hat{u}_h^1, \ldots, \hat{u}_h^m) \in U_h \text{ such that} \\ \qquad b(z_h, v_h) = l(v_h), \ \ \forall v_h \in V_h^{opt}, \end{cases} \tag{18}$$

being the trial-to-test operator $\Phi : U_h \longrightarrow V$ defined by

$$(\Phi z_h, v)_V = b(z_h, v), \ \forall v \in V, \ z_h \in U_h. \tag{19}$$

To compute the trial-to-test operator (19) in the presented setting, we solve the following problem: given a discrete trial function $z_h = (u_h, \hat{u}_h^1, \ldots, \hat{u}_h^m) \in U_h$, we solve

$$\begin{aligned} &\sum_{k=1}^{m} \int_{I_k} (-v' + \lambda v)(-(\delta v)' + \lambda \delta v)dt + [v]_k [\delta v]_k \\ &= \sum_{k=1}^{m} \int_{I_k} u_h(-(\delta v)' + \lambda \delta v)dt - \hat{u}_h^k [\delta v]_k, \ \forall \delta v \in V. \end{aligned} \tag{20}$$

Selecting in (20) test functions with local support in I_k, we obtain

$$\begin{aligned} &\int_{I_k} (-v' + \lambda v)(-(\delta v)' + \lambda \delta v)dt - [v]_k \delta v(t_k^-) + [v]_{k-1} \delta v(t_{k-1}^+) \\ &= \int_{I_k} u_h(-(\delta v)' + \lambda \delta v)dt + \hat{u}_h^k \delta v(t_k^-) - \hat{u}_h^{k-1} \delta v(t_{k-1}^+), \ \forall k = 1, \ldots, m, \end{aligned} \tag{21}$$

and solving the corresponding BVPs we have that

$$\Phi(u_h, \hat{u}_h^1, \dots, \hat{u}_h^m) = e^{\lambda t}\alpha_k + e^{\lambda t}\int_t^{t_k} e^{-\lambda\tau}u_h(\tau)d\tau,\ \forall t \in I_k,\ \forall k = 1, \dots, m \tag{22}$$

where

$$\begin{cases} \alpha_k = \alpha_{k+1} + e^{-\lambda t_k}\hat{u}_h^k + \int_{I_{k+1}} e^{-\lambda t}u_h(t)dt,\ \forall k = 1, \dots, m-1, \\ \alpha_m = e^{-\lambda t_m}\hat{u}_h^m, \end{cases}$$

or equivalently

$$\begin{cases} \alpha_k = \sum_{j=k}^{m} e^{-\lambda t_j}\hat{u}_h^j + \sum_{j=k}^{m-1}\int_{I_{j+1}} e^{-\lambda t}u_h(t)dt,\ \forall k = 1, \dots, m-1, \\ \alpha_m = e^{-\lambda t_m}\hat{u}_h^m. \end{cases}$$

For details of the proof of (22), see Appendix A.

Remark 3. Note that the optimal test function corresponding to each trace variable is

$$\Phi(0, 0, \dots, \underbrace{1}_{k+1}, \dots, 0) = e^{\lambda(t-t_k)},$$

and for the interiors, if we select a basis of $U_{h,0}$ as piecewise polynomials with local support over each element, we have that

$$\Phi(u_h, 0, \dots, 0) = e^{\lambda t}\int_t^{t_k} e^{-\lambda\tau}u_h(\tau)d\tau,\ \forall t \in I_k,\ \forall k = 1, \dots, m.$$

Therefore, the optimal test space of problem (18) is the span of the optimal test functions defined in Section 4 repeated at each element, i.e.,

$$V_h^{opt} = span\{\hat{v}^k, v_r^k,\ \forall r = 0, \dots, p,\ \forall k = 1, \dots, m\},$$

where $\hat{v}^k(\lambda, t) = e^{\lambda(t-t_k)},\ \forall t \in I_k$ and

$$\begin{aligned} v_r^k(\lambda, t) &= \frac{1}{\lambda}\left(\left(\frac{t-t_{k-1}}{h_k}\right)^r + \frac{r}{h_k}v_{r-1}^k(\lambda, t) - \hat{v}^k(\lambda, t)\right) \\ &= \frac{1}{\lambda^{r+1}h_k^r}\left(\mathcal{P}_r^k(\lambda, t) - \mathcal{P}_r^k(\lambda, t_k)\hat{v}^k(\lambda, t)\right),\ \forall t \in I_k. \end{aligned} \tag{23}$$

Here, $\mathcal{P}_r^k(\lambda, t)$ is a polynomial of order r defined as

$$\mathcal{P}_r^k(\lambda, t) = \sum_{j=0}^{r}\frac{r!}{j!}\lambda^j\left(t - t_{k-1}\right)^j,\ \forall t \in I_k.$$

In this case, optimal test functions (23) satisfy the following properties $\forall k = 1, \dots, m$

$$\begin{cases} -(\hat{v}^k(\lambda, t))' + \lambda\hat{v}^k(\lambda, t) = 0, \quad \hat{v}^k(\lambda, t_k) = 1, \\ -(v_r^k(\lambda, t))' + \lambda v_r^k(\lambda, t) = \left(\frac{t-t_{k-1}}{h_k}\right)^r, \quad v_r^k(\lambda, t_k) = 0,\ \forall r = 0, \dots, p, \end{cases}$$

and problem (18) reduces to the following time-marching scheme $\forall k = 1, \dots, m$

$$\begin{cases} \hat{u}_h^k = \hat{u}_h^{k-1}\hat{v}^k(\lambda, t_{k-1}) + \int_{I_k} f(t)\hat{v}^k(\lambda, t)dt, \\ \int_{I_k} u_h^k\left(\frac{t-t_{k-1}}{h_k}\right)^r dt = \hat{u}_h^{k-1}v_r^k(\lambda, t_{k-1}) + \int_{I_k} f(t)v_r^k(\lambda, t)dt,\ \forall r = 0, \dots, p, \end{cases} \tag{24}$$

where $\hat{u}_h^0 = u_0$ and $u_h^k(t)$ is the restriction $u_h(t)$ to interval I_k.

Remark 4. Note that if we restrict (24) to a single interval we obtain exactly (16). Therefore, we can: (a) formulate the DPG method for a single element and then use the resulting trace solution as the initial condition for the subsequent interval or (b) calculate the optimal test functions globally. With both settings ((a) and (b)) we obtain the same time-marching scheme and therefore, they deliver the same solution.

6. Linear ODE systems

We now consider the following linear system of ODEs

$$\begin{cases} u' + Au = f, & \text{in } I, \\ u(0) = u_0, \end{cases} \tag{25}$$

where $A \in \mathbb{R}^{n\times n}$ is a matrix that results from a spatial discretization of a linear parabolic Partial Differential Equation (PDE). Here, the solution and the source are vector functions $u, f : I \longrightarrow \mathbb{R}^n$, i.e.,

$$u(t) = (u_1(t), \dots, u_n(t))^T, \quad f(t) = (f_1(t), \dots, f_n(t))^T,$$

and similarly $u_0 = (u_{0,1}, \dots, u_{0,n})^T \in \mathbb{R}^n$. In this section, we denote as $||\cdot||$ the Euclidean norm of $\mathbb{R}^n$.

6.1. PG method with optimal test functions

Now, we formulate the ideal PG method for system (25). We define by $(\cdot,\cdot)$ the usual dot product in $\mathbb{R}^n$

$$(u, v) = u^T v,$$

and therefore $||\cdot||^2 = (\cdot,\cdot)$. Integrating by parts and employing that $(Au, v) = (u, A^T v)$, we write the variational formulation of (25) as

$$-\int_I (u, v')\, dt + \int_I (u, A^T v)\, dt + (\hat{u}, v(1)) = \int_I (f, v)\, dt + (u_0, v(0)).$$

Here, the trial and test spaces are $U = U_0 \times \hat{U} = L^2(I, \mathbb{R}^n) \times \mathbb{R}^n$ and $V = H^1(I, \mathbb{R}^n)$. We consider the following norms

$$||u||_U^2 = \int_I ||u||^2 dt + ||\hat{u}||^2,$$

$$||v||_V^2 = \int_I ||-v' + A^T v||^2 dt + ||v(1)||^2,$$

so the variational formulation of system (25) reads

$$\begin{cases} \text{Find } z = (u, \hat{u}) \in U \text{ such that} \\ \quad b(z, v) = l(v), \ \ \forall v \in V, \end{cases} \tag{26}$$

where

$$b(z, v) := -\int_I (u, v')\, dt + \int_I (u, A^T v)\, dt + (\hat{u}, v(1)),$$

$$l(v) := \int_I (f, v)\, dt + (u_0, v(0)).$$

Now, we calculate the optimal test functions of the ideal PG method. Given a subspace $U_h = U_{h,0} \times \hat{U} \subset U$ and a trial function $z_h = (u_h, \hat{u}_h) \in U_h$, we find $v \in V$ such that

$$(v, \delta v)_V = b(z_h, \delta v), \ \ \forall \delta v \in V, \tag{27}$$

which is equivalent to

$$\int_I (-v' + A^T v, -(\delta v)' + A^T \delta v) dt + (v(1), \delta v(1)) = \int_I (u_h, -(\delta v)' + A^T \delta v) dt + (\hat{u}_h, \delta v(1)).$$

Again, integrating by parts and applying Fourier's lemma, we obtain the following BVP

$$\begin{cases} -v'' + (A^T - A)v' + AA^T v = u_h' + Au_h, \\ -v'(0) + A^T v(0) = u_h(0), \\ v'(1) - A^T v(1) + v(1) = -u_h(1) + \hat{u}_h, \end{cases} \tag{28}$$

and following the same argument as in Remark 1, we can see that the solution of (28) is

$$\Phi(u, \hat{u}) = e^{A^T(t-1)}\hat{u}_h + e^{A^T t}\int_t^1 e^{-A^T\tau}u_h(\tau)d\tau. \tag{29}$$

6.2. Optimal test functions for polynomials of order p

We consider the discrete trial space $U_h = U_{h,0} \times \hat{U}$, where $U_{h,0}$ is composed of polynomials of order p. Then, we can express the solution $z_h = (u_h, \hat{u}_h) \in U_h$ of problem (5) as

$$u_h = \sum_{j=0}^{p} u_{h,j}t^j,$$

where in this case $u_{h,j} \in \mathbb{R}^n$ and also $\hat{u}_h \in \mathbb{R}^n$. As in Section 4, we calculate the optimal test functions.

6.2.1. Lowest order case ($p = 0$)

As for the 1D case, we first select $U_{h,0}$ as the space of constant functions in time and we denote by $\{\mathbf{e}_i\}_{i=1}^n$ the canonical basis of $\mathbb{R}^n$, i.e.,

$$\mathbf{e}_i = [0, \dots, 0, \underbrace{1}_{i}, 0, \dots, 0], \ \forall i = 1, \dots, n,$$

and $\mathbf{0} = [0, \dots, 0]$ the zero vector. In this case, we have

$$\begin{aligned} \hat{\mathbf{v}}_i(A^T, t) &:= \Phi(\mathbf{0}, \mathbf{e}_i) = e^{A^T(t-1)}\mathbf{e}_i, \\ \mathbf{v}_{0,i}(A^T, t) &:= \Phi(\mathbf{e}_i, \mathbf{0}) = e^{A^T t}\int_t^1 e^{-A^T\tau}\mathbf{e}_i d\tau = e^{A^T t}\left[(-A^T)^{-1}e^{-A^T\tau}\right]_t^1 \mathbf{e}_i \\ &= (A^T)^{-1}\left[I_n - e^{A^T(t-1)}\right]\mathbf{e}_i. \end{aligned}$$

Therefore, the optimal test space is $V_h^{opt} = span\left\{\hat{\mathbf{v}}_i, \mathbf{v}_{0,i}, \ \forall i = 1, \dots, n\right\}$. Here, the optimal test functions satisfy

$$\begin{cases} -\hat{\mathbf{v}}_i'(A^T, t) + A^T\hat{\mathbf{v}}_i(A^T, t) = \mathbf{0}, \quad \hat{\mathbf{v}}_i(A^T, 1) = \mathbf{e}_i, \quad \forall i = 1, \dots, n, \\ -\mathbf{v}_{0,i}'(A^T, t) + A^T\mathbf{v}_{0,i}(A^T, t) = \mathbf{e}_i, \quad \mathbf{v}_{0,i}(A^T, 1) = \mathbf{0}, \quad \forall i = 1, \dots, n. \end{cases}$$

Solving problem (5), we obtain the following method

$$\begin{cases} (\hat{u}_h, \mathbf{e}_i) = \left(u_0, \hat{\mathbf{v}}_i(A^T, 0)\right) + \int_0^1 \left(f(t), \hat{\mathbf{v}}_i(A^T, t)\right)dt, \ \forall i = 1, \dots, n, \\ (u_{h,0}, \mathbf{e}_i) = \left(u_0, \mathbf{v}_{0,i}(A^T, 0)\right) + \int_0^1 \left(f(t), \mathbf{v}_{0,i}(A^T, t)\right)dt, \ \forall i = 1, \dots, n. \end{cases} \tag{30}$$

6.2.2. Polynomials of order p

We can also calculate $\Phi(t^p\mathbf{e}_i, \mathbf{0})$ recursively as

$$\begin{aligned}\mathbf{v}_{p,i}(A^T,t) := \Phi(t^p\mathbf{e}_i,\mathbf{0}) &= e^{A^Tt}\int_t^1 e^{-A^T\tau}\tau^p\mathbf{e}_i d\tau\\ &= e^{A^Tt}\left(\left[-(A^T)^{-1}e^{A^T\tau}\tau^p\right]_t^1 + p(A^T)^{-1}\int_t^1 e^{-A^T\tau}\tau^{p-1}d\tau\right)\mathbf{e}_i\\ &= (A^T)^{-1}\left(t^pI_n - e^{A^T(t-1)} + pe^{A^Tt}\int_t^1 e^{-A^T\tau}\tau^{p-1}d\tau\right)\mathbf{e}_i,\end{aligned}$$

and equivalently

$$\mathbf{v}_{p,i}(A^T,t) = (A^T)^{-1}\left(t^p\mathbf{e}_i + p\mathbf{v}_{p-1,i}(A^T,t) - \hat{\mathbf{v}}_i(A^T,t)\right). \tag{31}$$

Here, $V_h^{opt} = span\{\hat{\mathbf{v}}_i, \mathbf{v}_{r,i},\ \forall r = 0,\dots,p,\ \forall i = 1,\dots,n\}$ and following the same steps as in Section 4.2, we can express (31) as

$$\mathbf{v}_{p,i}(A^T,t) = (A^T)^{-p-1}\left(\mathcal{P}_p(A^T,t) - \mathcal{P}_p(A^T,1)\hat{\mathbf{v}}(A^T,t)\right)\mathbf{e}_i, \tag{32}$$

where $\hat{\mathbf{v}}(A^T,t) = e^{A^T(t-1)}$ and $\mathcal{P}_p(A^T,t)$ is a polynomial of order p defined as

$$\mathcal{P}_p(A^T,t) = \sum_{j=0}^{p}\frac{p!}{j!}(A^Tt)^j.$$

Finally, the optimal test functions defined in (32) satisfy

$$-\mathbf{v}'_{p,i}(A^T,t) + A^T\mathbf{v}_{p,i}(A^T,t) = t^p\mathbf{e}_i, \quad \mathbf{v}_{p,i}(A^T,1) = \mathbf{0}, \quad \forall i = 1,\dots,n,$$

and we obtain the following scheme in problem (5)

$$\begin{cases}(\hat{u}_h,\mathbf{e}_i) = \left(u_0,\hat{\mathbf{v}}_i(A^T,0)\right) + \int_0^1\left(f(t),\hat{\mathbf{v}}_i(A^T,t)\right)dt,\ \forall i = 1,\dots,n,\\ \int_0^1\left(\sum_{j=0}^{p}u_{h,j}t^j, t^r\mathbf{e}_i\right)dt = \left(u_0,\mathbf{v}_{r,i}(A^T,0)\right) + \int_0^1\left(f(t),\mathbf{v}_{r,i}(A^T,t)\right)dt,\\ \qquad\forall r = 0,\dots,p,\ \forall i = 1,\dots,n.\end{cases} \tag{33}$$

In (33), we have $(p+1)n+n$ equations and $p+2$ unknowns that are vectors in $\mathbb{R}^n$. Therefore, we have a square system of $(p+2)n$ equations and $(p+2)n$ unknowns.

We express (33) in matrix form as

$$\begin{cases}\hat{u}_h^T = u_0^T\cdot\hat{\mathbf{v}}(A^T,0) + \int_0^1 f^T(t)\cdot\hat{\mathbf{v}}(A^T,t)dt,\\ \sum_{j=0}^{p}u_{h,j}^T\int_0^1 t^{j+r}dt = u_0^T\cdot\mathbf{v}_r(A^T,0) + \int_0^1 f^T(t)\cdot\mathbf{v}_r(A^T,t)dt,\ \forall r = 0,\dots,p,\end{cases} \tag{34}$$

where $\hat{\mathbf{v}}(A^T,t) = e^{A^T(t-1)}$ and

$$\begin{aligned}\mathbf{v}_r(A^T,t) &= (A^T)^{-1}\left(t^rI_n + r\mathbf{v}_{p-1}(A^T,t) - \hat{\mathbf{v}}(A^T,t)\right)\\ &= (A^T)^{-r-1}\left(\mathcal{P}_r(A^T,t) - \mathcal{P}_r(A^T,1)\hat{\mathbf{v}}(A^T,t)\right),\ \forall r = 0,\dots,p.\end{aligned}$$

7. Relation of ideal DPG method with exponential integrators

7.1. Exponential integrators for linear parabolic problems

The exponential integrators are a class of finite difference methods to discretize in time system (25) [29]. They are based on the fact that the analytical solution of the system can be expressed as

$$u(t) = e^{-At}u_0 + e^{-At}\int_0^t e^{A\tau} f(\tau)d\tau, \tag{35}$$

called variation-of-constants formula. Here, e^A is an exponential matrix defined as

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!},$$

and $A^0 = I_n$ is the identity matrix. Considering the partition defined in (17) and the variation-of-constants formula (35), we express the solution at each time step as

$$u(t_k) = e^{-h_k A}u(t_{k-1}) + \int_{t_{k-1}}^{t_k} e^{(\tau - t_k)A} f(\tau)d\tau. \tag{36}$$

In the exponential integrators, the integral in (36) is approximated using exponential quadrature rules. Selecting s quadrature points $c_i \in [0,1]$, $\forall i = 1,\dots,s$, we approximate the function $f(\tau)$ in (36) as

$$f(\tau) \approx \sum_{i=1}^{s} f(t_{k-1} + c_i h_k)\tilde{l}_i(\tau), \tag{37}$$

where $\tilde{l}_i(\tau)$ are the Lagrange basis polynomials defined at points $t_{k-1} + c_i h_k$, i.e.,

$$\tilde{l}_i(\tau) = \prod_{\substack{j=1\\ j\neq i}}^{s} \frac{\tau - (t_{k-1} + c_j h_k)}{(t_{k-1} + c_i h_k) - (t_{k-1} + c_j h_k)}, \ \forall i = 1,\dots,s.$$

We substitute (37) in (36), we integrate over the master element $[0,1]$, and we obtain the following expression

$$u^k = e^{-h_k A}u^{k-1} + h_k \sum_{i=1}^{s} b_i(-h_k A) f_i, \tag{38}$$

where $u^k \approx u(t_k)$, $\forall k = 0,\dots,m$, $f_i := f(t_{k-1} + c_i h_k)$, $\forall i = 1,\dots,s$ and the weights are defined as

$$b_i(z) = \int_0^1 e^{(1-\theta)z} l_i(\theta)d\theta, \ \forall i = 1,\dots,s, \tag{39}$$

where z could be a scalar value or a matrix and $l_i(\theta)$ are the Lagrange polynomials defined over the master element, i.e.,

$$l_i(\theta) = \prod_{\substack{j=1\\ j\neq i}}^{s} \frac{\theta - c_j}{c_i - c_j}, \ \forall i = 1,\dots,s.$$

In exponential integrators, the weights defined in (39) are usually given as linear combinations of the following functions

$$\begin{cases} \varphi_0(z) = e^z, \\ \varphi_p(z) = \displaystyle\int_0^1 e^{(1-\theta)z} \frac{\theta^{p-1}}{(p-1)!} d\theta, \ \forall p \geq 1, \end{cases} \tag{40}$$

which satisfy the following recurrence relation

$$\varphi_{p+1}(z) = \frac{1}{z}\left(\varphi_p(z) - \frac{1}{p!}\right). \tag{41}$$

Examples:

- If we select one point $c_1 \in [0,1]$, we have that $l_1(\theta) = 1$ and $b_1(z) = \varphi_1(z)$. Employing from (41) that $e^z = z\varphi_1(z) + 1$, we obtain the following method

$$u^k = u^{k-1} + h_k \varphi_1(-h_k A)\left(f_1 - Au^{k-1}\right). \tag{42}$$

If we select $c_1 = 0$, it is called exponential Euler method and when $c_1 = \frac{1}{2}$, exponential midpoint rule.

- If we select two points $c_1, c_2 \in [0,1]$, we have that

$$b_1(z) = \frac{1}{c_1 - c_2}\varphi_2(z) - \frac{c_2}{c_1 - c_2}\varphi_1(z),$$
$$b_2(z) = \frac{1}{c_2 - c_1}\varphi_2(z) - \frac{c_1}{c_2 - c_1}\varphi_1(z),$$

so we obtain the following scheme

$$\begin{aligned} u^k = u^{k-1} &- h_k A\varphi_1(-h_k A)u^{k-1} \\ &+ h_k\left(\frac{1}{c_1 - c_2}\varphi_2(-h_k A) - \frac{c_2}{c_1 - c_2}\varphi_1(-h_k A)\right) f_1 \\ &+ h_k\left(\frac{1}{c_2 - c_1}\varphi_2(-h_k A) - \frac{c_1}{c_2 - c_1}\varphi_1(-h_k A)\right) f_2, \end{aligned} \tag{43}$$

and selecting $c_1 = 0$ and $c_2 = 1$, we obtain the so-called exponential trapezoidal rule.

7.2. Ideal DPG as an exponential integrator

In the DPG methods defined in (16) and (33), the equations corresponding to the trace variables are equivalent to the transpose of the exponential integrator defined in (36). This is because we can express the equation of the trace variables in (34) as

$$\hat{u}_h = \hat{\mathbf{v}}(A,0)u_0 + \int_0^1 \hat{\mathbf{v}}(A,t)f(t)dt.$$

Therefore, we can solve the trace variables employing the classical exponential quadrature defined in (38).

Now, we can employ the approximation presented in Section 7.1 to calculate the interior variables in (16) and (33). For simplicity, we focus on approximating the right-hand-side of (16) in the master element. Employing (37), we have

$$\int_0^1 v_r(z,t)f(t)dt \approx \sum_{i=1}^{s} f(c_i)\int_0^1 v_r(z,t)l_i(t)dt, \ \forall r = 0,\dots,p, \tag{44}$$

where z is a scalar value (or a matrix). Clearly, the weights defined in (44) are linear combinations of $\int_0^1 v_r(z,t)t^q dt$, $\forall q = 0,\dots,s$. In order to present the method in terms of the functions defined in (40), we prove the following relations between those functions and the optimal test functions from the DPG method (the proof is given in Appendix A)

$$v_r(z,0) = \sum_{j=0}^{r}\frac{r!}{j!}(-1)^{r-j}\varphi_{r-j+1}(-z), \tag{45a}$$

$$\int_0^1 v_r(z,t)t^q dt = q!\sum_{j=0}^{r}\frac{r!}{j!}(-1)^{r-j}\varphi_{r-j+q+2}(-z). \tag{45b}$$

In (24) we integrate over the master element $[0,1]$. Then, we employ the following relations

$$\hat{v}^k(z, t_{k-1} + \theta h_k) = \hat{v}(zh_k, \theta),$$
$$v_r^k(z, t_{k-1} + \theta h_k) = h_k v_r(zh_k, \theta), \ \forall r = 0,\dots,p,$$

where $\hat{v}(z,t)$ and $v_r(z,t)$ are the optimal test functions defined over $[0,1]$.

Examples:

- For $p=0$ and one integration point $c_1 \in [0,1]$, we obtain (42) for the trace variables. For the interior, we have $v_0(z,0) = \varphi_1(-z)$ and $\int_0^1 v_0(z,t)dt = \varphi_2(-z)$. Therefore, the DPG method with piecewise constant trial functions becomes

$$\begin{aligned}\hat{u}_h^k &= \hat{u}_h^{k-1} + h_k\varphi_1(-h_kA)\left(f_1 - A\hat{u}_h^{k-1}\right),\\ u_{h,0}^k &= \varphi_1(-h_kA)\hat{u}_h^{k-1} + h_k\varphi_2(-h_kA)f_1.\end{aligned}$$

- For $p=1$ and two integration points $c_1, c_2 \in [0,1]$, we obtain (43) for the trace variables. The DPG method with piecewise linear trial functions becomes

$$\begin{aligned}\hat{u}_h^k = \hat{u}_h^{k-1} &- h_kA\varphi_1(-h_kA)\hat{u}_h^{k-1}\\ &+ h_k\left(\frac{1}{c_1-c_2}\varphi_2(-h_kA) - \frac{c_2}{c_1-c_2}\varphi_1(-h_kA)\right)f_1\\ &+ h_k\left(\frac{1}{c_2-c_1}\varphi_2(-h_kA) - \frac{c_1}{c_2-c_1}\varphi_1(-h_kA)\right)f_2,\end{aligned}$$

$$\begin{aligned}u_{h,0}^k + \frac{1}{2}u_{h,1}^k &= \varphi_1(-h_kA)\hat{u}_h^{k-1}\\ &+ h_k\left(\frac{1}{c_1-c_2}\varphi_3(-h_kA) - \frac{c_2}{c_1-c_2}\varphi_2(-h_kA)\right)f_1\\ &+ h_k\left(\frac{1}{c_2-c_1}\varphi_3(-h_kA) - \frac{c_1}{c_2-c_1}\varphi_2(-h_kA)\right)f_2,\\ \frac{1}{2}u_{h,0}^k + \frac{1}{3}u_{h,1}^k &= \varphi_1(-h_kA)\hat{u}_h^{k-1} - \varphi_2(-h_kA)\hat{u}_h^{k-1}\\ &+ h_k\left(\frac{1}{c_1-c_2}(\varphi_3(-h_kA) - \varphi_4(-h_kA))\right.\\ &\qquad\left. - \frac{c_2}{c_1-c_2}(\varphi_2(-h_kA) - \varphi_3(-h_kA))\right)f_1\\ &+ h_k\left(\frac{1}{c_2-c_1}(\varphi_3(-h_kA) - \varphi_4(-h_kA))\right.\\ &\qquad\left. - \frac{c_1}{c_2-c_1}(\varphi_2(-h_kA) - \varphi_3(-h_kA))\right)f_2.\end{aligned}$$

8. Numerical results

In this section, we present the performance of the method presented in (24) for a single ODE and a system of ODEs coming from parabolic PDEs. For the discretization in space, we employ the FEM with piecewise linear functions. For the computation of the φ-functions defined in (40), we employ the MATLAB package called *EXPINT* presented in [4] that employs Padé approximations.

Example 1. We consider the first order ODE (1) where the exact solution is

$$u(t) = \frac{e^{M(t-1)} - e^{-M}}{1 - e^{-M}}.$$

In this case, the source term is constant $f(t) = \dfrac{M}{e^M - 1}$ and we set $M = 15$, $\lambda = -M$ and $I = (0,1]$. Fig. 2 shows the exact and the DPG solutions solving (24) for $p=0$, $p=1$ and $p=2$. Fig. 3 illustrates the convergence of the error and Table 1 shows that the convergence rates are $p+1$.

Example 2. We now consider the same solution as in Example 1 but with $\lambda = -1$. In this case, the source term depends on time

$$f(t) = \frac{e^{Mt}(M+\lambda) - \lambda}{e^M - 1}.$$

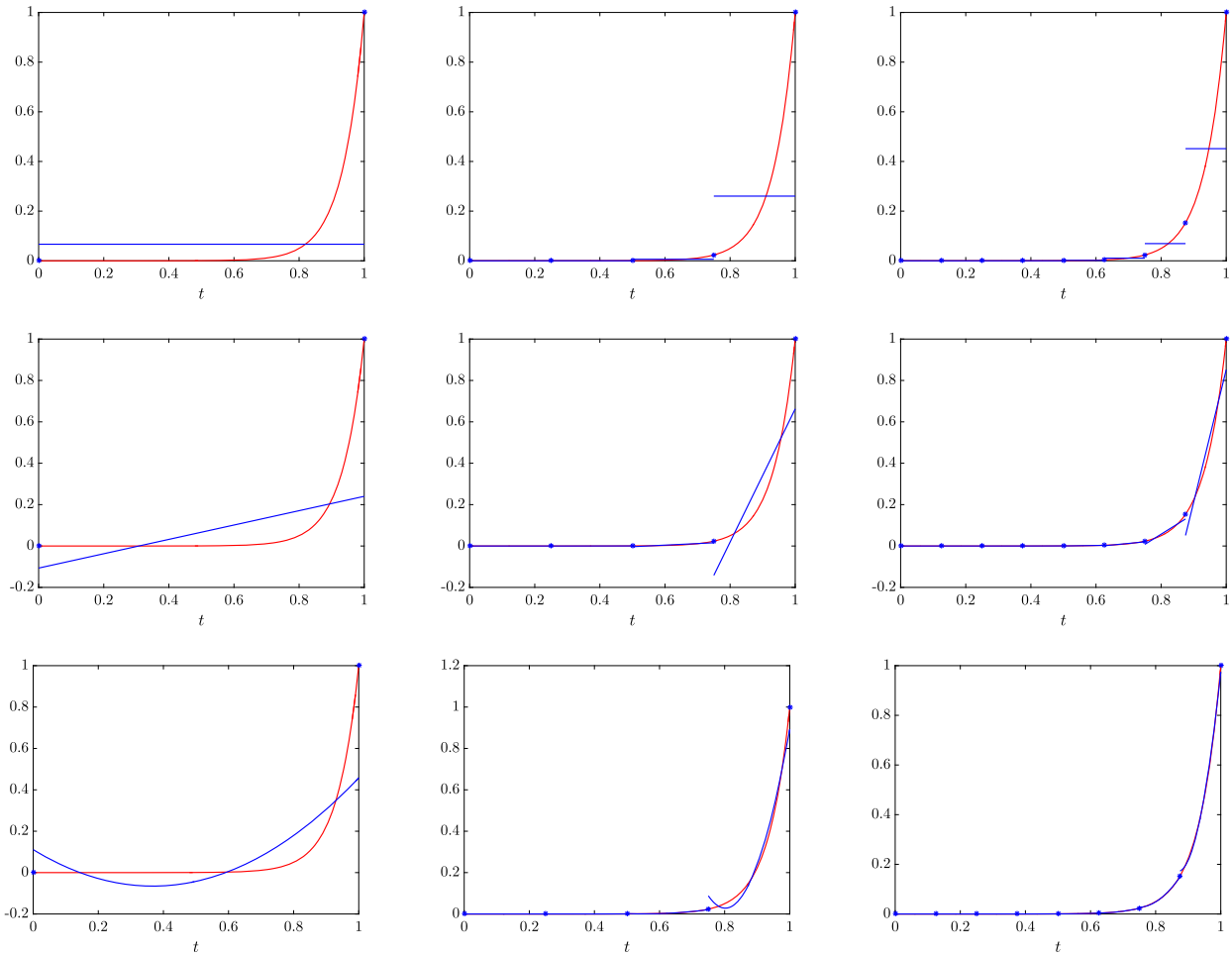


Fig. 2. Approximated solution of Example 1 for $p = 0$ (first row), $p = 1$ (second row) and $p = 2$ (third row). (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

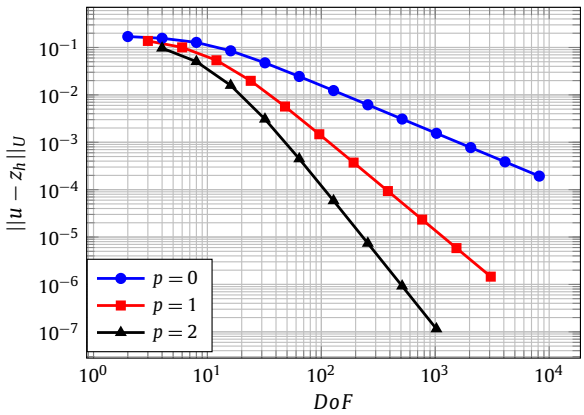


Fig. 3. Convergence of the error for $p = 0$, $p = 1$ and $p = 2$ of Example 1.

Table 1
Convergence rates for $p = 0$, $p = 1$ and $p = 2$ of Example 1.

$p = 0$	$p = 1$	$p = 2$
0.1202	0.4520	0.9448
0.2894	0.9026	1.6675
0.5893	1.4415	2.3655
0.8441	1.8013	2.7808
0.9550	1.9438	2.9386
0.9883	1.9855	2.9841
0.9970	1.9963	2.9960
0.9993	1.9991	3.0020
0.9998	1.9998	
1.0000	1.9999	
1.0000		
1.0000		

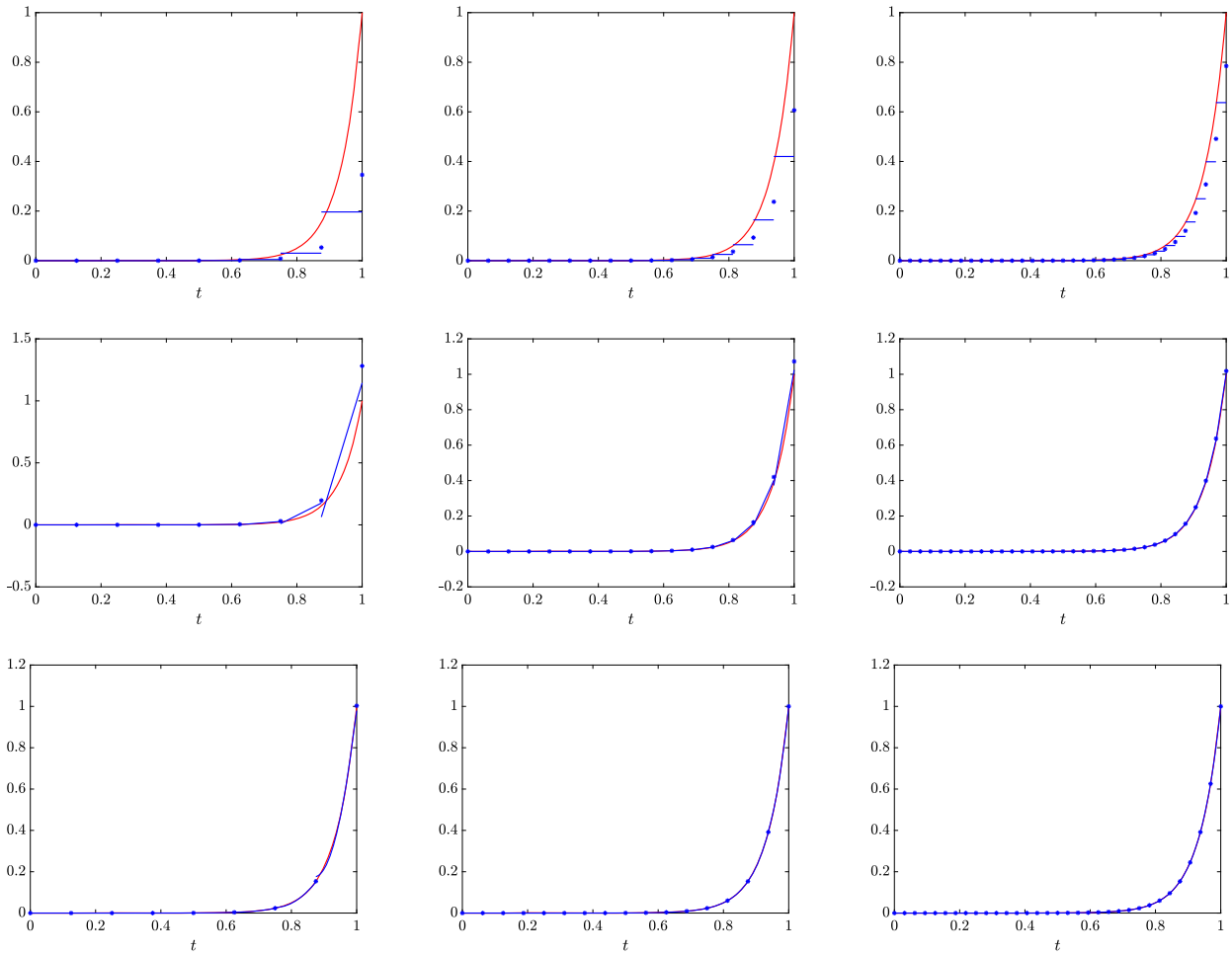


Fig. 4. Approximated solution of Example 2 for $p = 0$ (first row), $p = 1$ (second row) and $p = 2$ (third row).

Figs. 4 and 5 show the approximated solutions and the convergence of the error for p up to 2, respectively. We observe that the convergence rates are 0.5, 1.5, and 3 for $p = 0$, $p = 1$, and $p = 2$, respectively. The reason is that the approximation of the source term for $p = 0$ and $p = 1$ is not sufficient to obtain a convergence rate of $p + 1$ (Table 2).

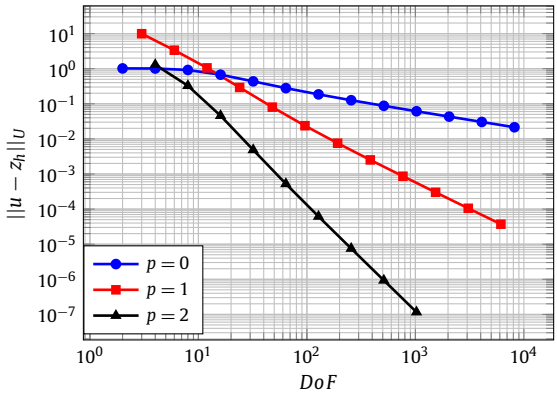


Fig. 5. Convergence of the error for $p = 0$, $p = 1$ and $p = 2$ of Example 2.

Table 2
Convergence rates for $p = 0$, $p = 1$ and $p = 2$ of Example 2.

$p = 0$	$p = 1$	$p = 2$
0.0072	1.5600	1.9889
0.1382	1.6731	2.8341
0.4485	1.8525	3.2378
0.6310	1.8635	3.2102
0.6386	1.7586	3.0909
0.5936	1.6535	3.0328
0.5539	1.5836	3.0124
0.5289	1.5437	3.0051
0.5150	1.5223	
0.5076	1.5113	
0.5038	1.5057	
0.5019		

Table 3
Convergence rates for $p = 0$, $p = 1$ and $p = 2$ of Example 3.

$p = 0$	$p = 1$	$p = 2$
0.4628	1.2366	2.1138
0.7609	1.6895	2.6546
0.9249	1.9058	2.8967
0.9799	1.9750	2.9655
0.9949	1.9935	
0.9987	1.9936	
0.9997		

Example 3. We consider the heat equation

$$\begin{cases} \dfrac{\partial u}{\partial t} - \alpha^2 \dfrac{\partial^2 u}{\partial x^2} = f(x,t), & \forall (x,t) \in \Omega \times I, \\ u(x,t) = 0, & \forall (x,t) \in \partial\Omega \times I, \\ u(x,0) = u_0(x), & \forall x \in \Omega, \end{cases} \tag{46}$$

where $\Omega = (0,1)$, $I = (0, 0.5]$, $\alpha = 1$, $f = 0$ and $u_0(x) = \sin(\pi x)$. The exact solution of problem (46) is

$$u(x,t) = e^{-\pi^2 t} sin(\pi x).$$

We discretize the space variable using a FEM with piecewise linear basis functions to obtain a system of the form (25). In this case, $A = M^{-1}K$ where M and K are the mass and stiffness matrices from the FEM discretization, respectively. Figs. 6 and 7 illustrate the approximated solutions with a mesh in space of 600 elements. Fig. 8 shows the convergence of the error for uniform time refinements. We observe in Table 3 convergence rates of $p + 1$.

Example 4. Transient Eriksson-Johnson problem. We consider the following 2D + time advection-diffusion problem that is similar to the one introduced in [18]

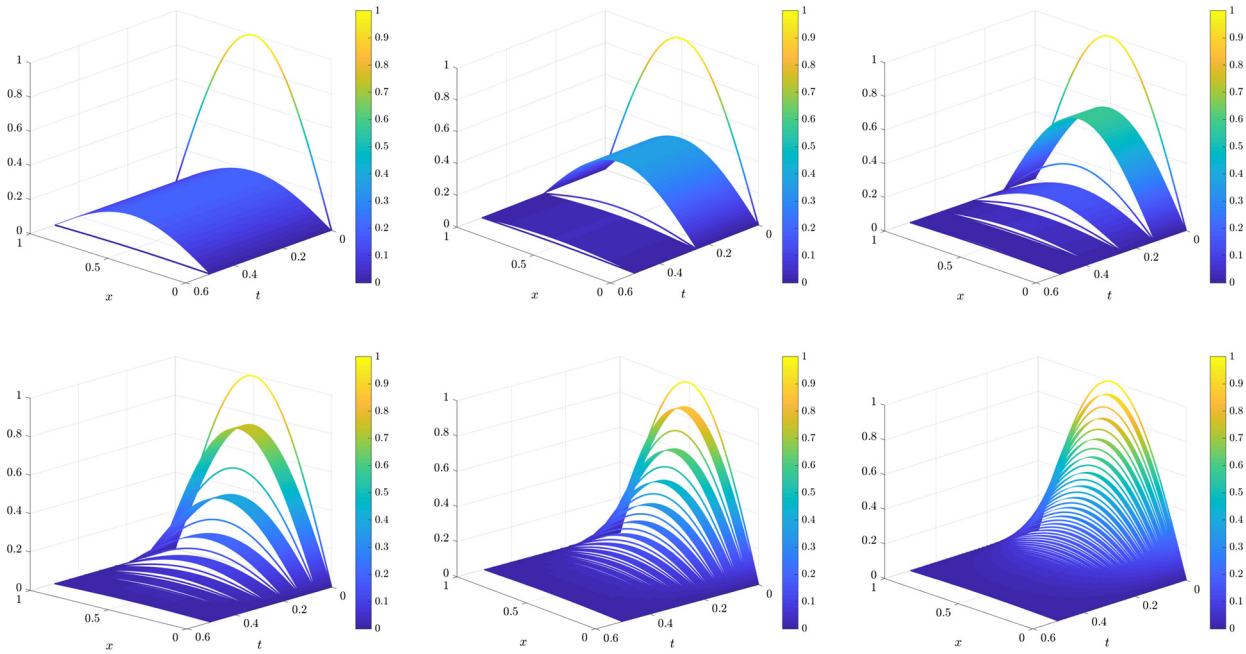


Fig. 6. Approximated solution of Example 3 for $p = 0$.

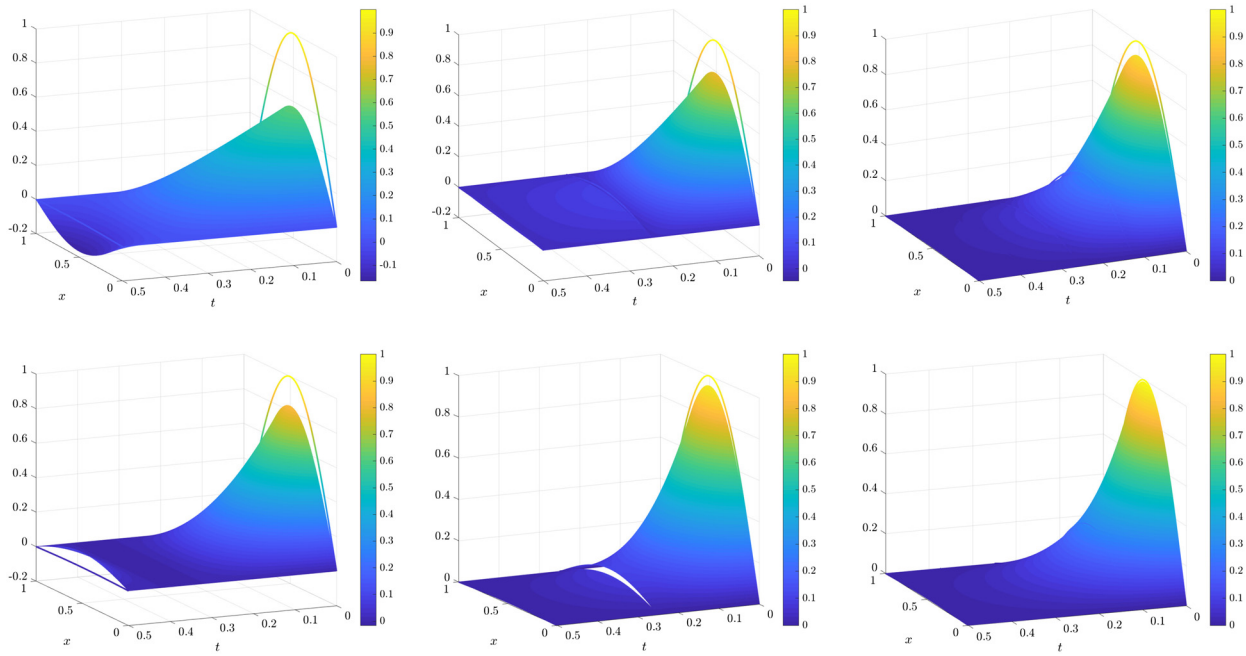


Fig. 7. Approximated solution of Example 3 for $p = 1$ (first row) and $p = 2$ (second row).

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} - \epsilon \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = f(x, y, t),$$

over $\Omega = (-1, 0) \times (-0.5, 0.5)$ and $I = (0, 1]$. We select the data of the problem in such a way that the exact solution is

$$u(x, y, t) = Ce^{-lt} x \left(y^2 - 0.25 \right) + \frac{e^{r_1 x} - e^{r_2 x}}{e^{-r_1} - e^{-r_2}} \cos(\pi y),$$

where $r_{1,2} = \dfrac{1 \pm \sqrt{4\pi^2 \epsilon^2}}{2\epsilon}$. Therefore, we have

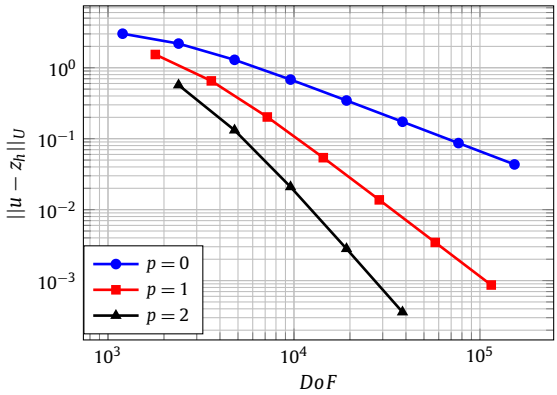
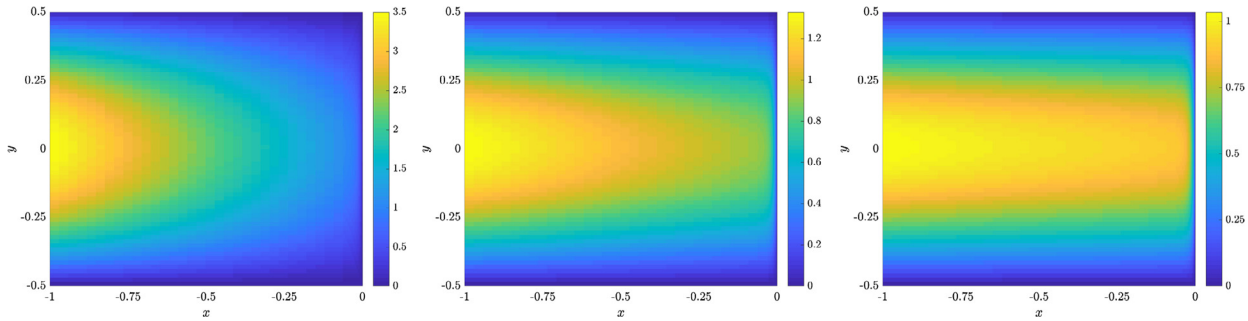


Fig. 8. Convergence of the error for $p = 0$, $p = 1$ and $p = 2$ of Example 3.



(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1$

Fig. 9. Approximated solution of Example 4 for $p = 2$.

$$f(x, y, t) = Ce^{-lt}\left((y^2 - 0.25)(1 - lx) - 2\epsilon x\right),$$

and the following boundary and initial conditions

$$\begin{cases} \dfrac{\partial}{\partial x}u(-1, y, t) = Ce^{-lt}\left(y^2 - 0.25\right) + \dfrac{r_1 e^{-r_1} - r_2 e^{-r_2}}{e^{-r_1} - e^{-r_2}}\cos(\pi y), \\ u(0, y, t) = u(x, -0.5, t) = u(x, 0.5, t) = 0, \\ u(x, y, 0) = Cx\left(y^2 - 0.25\right) + \dfrac{e^{r_1 x} - e^{r_2 x}}{e^{-r_1} - e^{-r_2}}\cos(\pi y). \end{cases}$$

The solution has a boundary layer at $x = 0$ and it decays to the solution of the stationary Eriksson-Johnson problem [21]. We set $C = 10$, $l = 4$ and $\epsilon = 10^{-2}$. For the space discretization, we select a non-uniform mesh with 2^6 elements per space dimension. Fig. 9 shows some colormaps of the approximated solution for different time steps. Finally, Fig. 10 presents the following relative error in percentage

$$\frac{||u - z_h||_U}{||u||_U} \cdot 100.$$

We observe that the error remains constant after some refinements in time due to the discretization error in space.

9. Conclusions

In this work, we apply the DPG method for the time integrations of linear systems of first order ODEs. We prove that applying the DPG method for a single interval and using the resulting trace variable as initial condition for the next interval is equivalent to the scheme obtained after applying the DPG method globally. For parabolic problems, the DPG method in time is equivalent to the exponential integrators for the trace variables. In addition, the DPG method provides the element interiors, which can be locally computed. We express the resulting DPG-based time-marching scheme in terms of the φ-functions in order to employ the software available from the exponential integrators community. For piecewise polynomials of order p in time for the trial space, we need $p + 1$ φ-functions to calculate the traces and $2p + 2$ φ-functions to compute

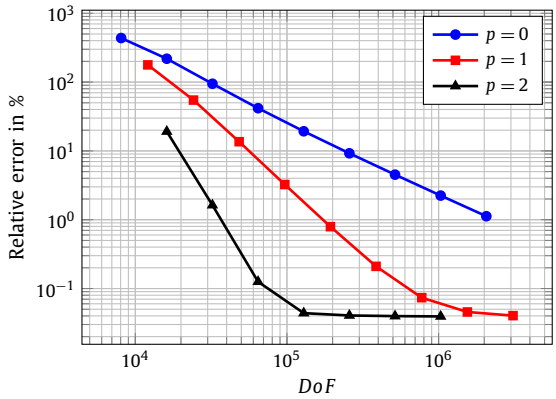


Fig. 10. Relative error in percentage for $p=0$, $p=1$ and $p=2$ of Example 4.

the interiors. This DPG based time-marching scheme can be combined with any other discretization in space for linear parabolic PDEs.

Possible extensions of this work include: (a) the fast computation of element interiors; (b) application of the proposed DPG method to linear hyperbolic problems and nonlinear parabolic equations; (c) to consider a space discretization obtained with DPG; and (d) the use of adaptive strategies and a posteriori error estimation.

CRediT authorship contribution statement

Judit Muñoz-Matute: Formal analysis, Investigation, Software, Validation, Writing – original draft. **David Pardo:** Funding acquisition, Supervision, Writing – review & editing. **Leszek Demkowicz:** Resources, Supervision, Writing – review & editing.

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.

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Appendix A. Proofs

Proof of (10)$\Longleftrightarrow$(8).

- (10)$\Longrightarrow$(8): We differentiate the first equation of (10) and we add it to the first equation of (10) multiplied by λ to obtain the first equation of (8). We obtain the second equation of (8) by evaluating the first equation of (10) at 0. Finally, evaluating the first equation of (10) at T and adding it to the second equation of (10), we obtain the third equation of (8).
- (8)$\Longrightarrow$(10): We employ the function $y=e^{\lambda t}$ that satisfies $y'=\lambda y$ and $y''=\lambda^2 y$. If we multiply the first equation of (8) by y, we obtain

$$-v''y+vy''=u_h'y+u_hy',$$

or equivalently $(vy' - v'y)' = (u_h y)'$. Integrating over $(0, t)$ we obtain

$$v(t)y'(t) - v'(t)y(t) - v(0)y'(0) + v'(0)y(0) = u_h(t)y(t) - u_h(0)y(0),$$

and equivalently

$$(-v'(t) + \lambda v(t))y(t) + (v'(0) - \lambda v(0))y(0) = u_h(t)y(t) - u_h(0)y(0).$$

From the second equation of (8), the terms at 0 vanish and therefore $-v'(t) + \lambda v(t) = u_h(t)$ which is the first equation of (10). Finally, we have that $-v'(1) + \lambda v(1) = u_h(1)$ and from the third equation of (8) we obtain $v(1) = \hat{u}_h$. □

Proof of equation (14). We employ an induction argument $\forall p \geq 0$.

- We first prove equality (14) for $p = 0$. We have that

$$\mathcal{P}_0(\lambda, t) = 1, \quad \hat{v}(\lambda, t) = e^{\lambda(t-1)}, \text{ and } v_0(\lambda, t) = \frac{1}{\lambda}(1 - e^{\lambda(t-1)}).$$

- We suppose that (14) holds for $p - 1$, i.e.,

$$v_{p-1}(\lambda, t) = \frac{1}{\lambda^p}\left(\mathcal{P}_{p-1}(\lambda, t) - \mathcal{P}_{p-1}(\lambda, 1)\hat{v}(\lambda, t)\right), \tag{A.1}$$

where $\mathcal{P}_{p-1}(\lambda, t) = \sum_{j=0}^{p-1} \frac{(p-1)!}{j!}(\lambda t)^j$ and we prove (14) for $v_p(\lambda, t)$. Note that

$$p\mathcal{P}_{p-1}(\lambda, t) + (\lambda t)^p = \sum_{j=0}^{p-1} \frac{p(p-1)!}{j!}(\lambda t)^j + (\lambda t)^p = \sum_{j=0}^{p} \frac{p!}{j!}(\lambda t)^j = \mathcal{P}_p(\lambda, t). \tag{A.2}$$

We express (A.1) as

$$\begin{aligned} p v_{p-1}(\lambda, t) = \frac{1}{\lambda^p}\big(&p\mathcal{P}_{p-1}(\lambda, t) + (\lambda t)^p - (\lambda t)^p - p\mathcal{P}_{p-1}(\lambda, 1)\hat{v}(\lambda, t) \\ &+\lambda^p \hat{v}(\lambda, t) - \lambda^p \hat{v}(\lambda, t)\big), \end{aligned}$$

from (A.2) we obtain

$$p v_{p-1}(\lambda, t) = \frac{1}{\lambda^p}(\mathcal{P}_p(\lambda, t) - (\lambda t)^p - \mathcal{P}_p(\lambda, 1)\hat{v}(\lambda, t) + \lambda^p \hat{v}(\lambda, t)),$$

and equivalently

$$t^p + p v_{p-1}(\lambda, t) - \hat{v}(\lambda, t) = \frac{1}{\lambda^p}(\mathcal{P}_p(\lambda, t) - \mathcal{P}_p(\lambda, 1)\hat{v}(\lambda, t)).$$

Finally, from (13) we obtain

$$v_p(\lambda, t) = \frac{1}{\lambda^{p+1}}(\mathcal{P}_p(\lambda, t) - \mathcal{P}_p(\lambda, 1)\hat{v}(\lambda, t)). \quad \square$$

Proof of equation (22). Following an analogue argument to the one employed in Remark 1, we conclude that problem (21) is equivalent to the following BVPs

$$\begin{cases} -v_k' + \lambda v_k = u_h, \ \forall t \in I_k, \\ v_k(t_{k-1}^+) - v_{k-1}(t_{k-1}^-) = -\hat{u}_h^{k-1}, \\ -v_{k+1}(t_k^-) + v_k(t_k^-) = \hat{u}_h^k, \end{cases} \tag{A.3}$$

where we denote with $v_k(t)$ the restriction of $v(t)$ to I_k. In (A.3), we have m overlapping BVPs. From the first equation of (A.3), we have that

$$v_k(t) = \alpha_k e^{\lambda t} + e^{\lambda t} \int_t^{t_k} e^{-\lambda \tau} u_h(\tau) d\tau, \ \forall t \in I_k, \ \forall k = 1, \ldots, m.$$

From the second and third equations of (A.3), we obtain

$$\alpha_k e^{\lambda t_k} = \hat{u}_h^k + \alpha_{k+1} e^{\lambda t_k} + e^{\lambda t_k} \int_{t_k}^{t_{k+1}} e^{-\lambda s} u_h(s) ds, \ \forall k = 1, \ldots, m-1. \tag{A.4}$$

For $k = m$, the third equation of (A.3) reduces to $v_m(t_m^-) = \hat{u}_h^m$, i.e.,

$$\alpha_m e^{\lambda t_m} = \hat{u}_h^m. \tag{A.5}$$

Finally, from equations (A.4) and (A.5) we obtain (22). □

Proof of equation (45a). We employ and induction argument for $r \geq 0$.

- We first prove (45a) for $r = 0$: From (11) and (41), we have that

$$v_0(z, 0) = \frac{1}{z}\left(1 - e^{-z}\right) = \frac{1}{-z}\left(e^{-z} - 1\right) = \varphi_1(-z).$$

- We suppose (45a) is true for $r - 1$:

$$v_{r-1}(z, 0) = \sum_{j=0}^{r-1} \frac{(r-1)!}{j!} (-1)^{r-j-1} \varphi_{r-j}(-z) \tag{A.6}$$

- We prove (45a) for r: We employ recursive relations (13) and (41), the induction hypothesis (A.6) and, definitions (11) and (40). Therefore, we obtain

$$\begin{aligned}
v_r(z, 0) &= \frac{1}{z}\left(r v_{r-1}(z, 0) - \hat{v}(z, 0)\right) \\
&= \frac{r}{z} \sum_{j=0}^{r-1} \frac{(r-1)!}{j!} (-1)^{r-j-1} \varphi_{r-j}(-z) - \frac{1}{z} e^{-z} \\
&= \frac{1}{z} \sum_{j=0}^{r} \frac{r!}{j!} (-1)^{r-j-1} \varphi_{r-j}(-z) \\
&= \frac{1}{z} \sum_{j=0}^{r-1} \frac{r!}{j!} (-1)^{r-j-1} \left(\frac{1}{(r-j)!} - z\varphi_{r-j+1}(-z) \right) \\
&= \frac{1}{z} \left(\sum_{j=0}^{r} \frac{r!}{j!(r-j)!} (-1)^{r-j-1} \right) + \sum_{j=0}^{r} \frac{r!}{j!} (-1)^{r-j} \varphi_{r-j+1}(-z).
\end{aligned}$$

We just need to prove that the first term of the previous equation vanishes

$$\begin{aligned}
&\sum_{j=0}^{r} \binom{r}{j} (-1)^{r-j-1} = (-1)^{r-1} - 1 + \sum_{j=1}^{r-1} \left[\binom{r-1}{j} + \binom{r-1}{j-1} \right] (-1)^{r-j-1} \\
&= (-1)^{r-1} - 1 - \sum_{j=1}^{r-1} \binom{r-1}{j} (-1)^{r-j} + \sum_{j=0}^{r-2} \binom{r-1}{j} (-1)^{r-j} \\
&= (-1)^{r-1} - 1 + 1 - \sum_{j=1}^{r-2} \binom{r-1}{j} (-1)^{r-j} + \sum_{j=1}^{r-2} \binom{r-1}{j} (-1)^{r-j} + (-1)^r = 0.
\end{aligned}$$

□

Proof of equation (45b). We employ a double induction argument for $r \geq 0$ and $q \geq 0$.

- Induction over r, $\forall q \geq 0$:

– We first prove (45b) for $r=0$, $\forall q \geq 0$: We employ the definitions (11) and (40) and the recurrence formula (41)

$$\int_0^1 v_0(z,t)t^q dt = \frac{1}{z}\int_0^1 (1-e^{(t-1)z})t^q dt = \frac{1}{z}\left(\frac{1}{q+1} - q!\varphi_{q+1}(-z)\right)$$
$$= \frac{1}{z}\left(\frac{1}{q+1} - q!\left(\frac{1}{(q+1)!} - z\varphi_{q+2}(-z)\right)\right) = q!\varphi_{q+2}(-z).$$

– We suppose (45b) is true for $r-1$, $\forall q \geq 0$:

$$\int_0^1 v_{r-1}(z,t)t^q dt = q!\sum_{j=0}^{r-1}\frac{(r-1)!}{j!}(-1)^{r-j-1}\varphi_{r-j+q+1}(-z). \tag{A.7}$$

– We prove (45b) for r, $\forall q \geq 0$: Here we employ definition (40), the recurrence formulas (13) and (41) and the induction hypothesis (A.7)

$$\int_0^1 v_r(z,t)t^q dt = \frac{1}{z}\int_0^1 t^{r+q}dt + \frac{r}{z}\int_0^1 v_{r-1}(z,t)t^q dt - \frac{1}{z}\int_0^1 e^{z(t-1)}t^q dt$$
$$= \frac{1}{z}\frac{1}{r+q+1} + \frac{q!}{z}\sum_{j=0}^{r}\frac{r!}{j!}(-1)^{r-j-1}\varphi_{r-j+q+1}(-z)$$
$$= \frac{1}{z}\left(\frac{1}{r+q+1} + q!\sum_{j=0}^{r}\frac{r!(-1)^{r-j-1}}{j!(r-j+q+1)!}\right) + q!\sum_{j=0}^{r}\frac{r!}{j!}(-1)^{r-j}\varphi_{r-j+q+2}(-z).$$

We just need to prove that the first term in the previous equation vanishes

$$\begin{aligned}
&\frac{1}{r+q+1} + q!\sum_{j=0}^{r}\frac{r!}{j!(r-j+q+1)!}(-1)^{r-j-1}\\
&= \frac{1}{r+q+1} + \frac{q!r!}{(r+q+1)!}\sum_{j=1}^{r}\binom{q+r+1}{j}(-1)^{r-j-1} + (-1)^{r-1}\frac{q!r!}{(r+q+1)}\\
&= \frac{1}{r+q+1} + (-1)^{r-1}\frac{q!r!}{(r+q+1)}\\
&+ \frac{q!r!}{(r+q+1)!}\left[\sum_{j=1}^{r}\binom{q+r}{j}(-1)^{r-j-1} + \sum_{j=1}^{r}\binom{q+r}{j-1}(-1)^{r-j-1}\right]\\
&= \frac{1}{r+q+1} + (-1)^{r-1}\frac{q!r!}{(r+q+1)}\\
&+ \frac{q!r!}{(r+q+1)!}\left[-\frac{(q+r)!}{q!r!} - \sum_{j=1}^{r-1}\binom{q+r}{j}(-1)^{r-j} + \sum_{j=1}^{r-1}\binom{q+r}{j}(-1)^{r-j} + (-1)^r\right]\\
&= \frac{1}{r+q+1} - (-1)^r\frac{q!r!}{(r+q+1)} - \frac{1}{r+q+1} + (-1)^r\frac{q!r!}{(r+q+1)} = 0.
\end{aligned} \tag{A.8}$$

• Induction over q, $\forall r \geq 0$:

– To prove that (45b) is true for $q=0$, $\forall r \geq 0$, we can repeat the previous induction argument with $q=0$.
– We suppose (45b) is true for $q-1$, $\forall r \geq 0$:

$$\int_0^1 v_r(z,t)t^{q-1}dt = (q-1)!\sum_{j=0}^{r}\frac{r!}{j!}(-1)^{r-j}\varphi_{r-j+q+1}(-z). \tag{A.9}$$

– We prove (45b) for q, $\forall r \geq 0$: We employ property (15) and also $v_r(z,1) = 0$, $\forall r \geq 0$. Integrating by parts we obtain

$$\int_0^1 v_k(z,t)t^q dt = \frac{1}{z}\left(\int_0^1 v_r'(z,t)t^q dt + \int_0^1 t^{r+q} dt\right)$$
$$= \frac{1}{z}\frac{1}{r+q+1} - \frac{q}{z}\int_0^1 v_r(z,t)t^{q+1} dt.$$

From the induction hypothesis (A.9) and the recurrence formula (41), we have

$$\int_0^1 v_k(z,t)t^q dt = \frac{1}{z}\frac{1}{r+q+1} - \frac{q!}{z}\sum_{j=0}^{r}(-1)^{r-j}\varphi_{r-j+q+1}(-z)$$
$$= \frac{1}{z}\left(\frac{1}{r+q+1} - q!\sum_{j=0}^{r}\frac{r!}{j!}(-1)^{r-j}\frac{1}{(r-j+q+1)!}\right)$$
$$+ q!\sum_{j=0}^{r}\frac{r!}{j!}(-1)^{r-j}\varphi_{j-r+q+2}(-z).$$

Finally, we know from (A.8) that the first term in the previous equation vanishes and we obtain

$$\int_0^1 v_k(z,t)t^q dt = q!\sum_{j=0}^{r}\frac{r!}{j!}(-1)^{r-j}\varphi_{j-r+q+2}(-z). \quad \square$$

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