DPG time-marching scheme with DPG semidiscretization in space for transient advection-reaction equations

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MINRES/LS-5 October 5-7 Three approaches to discretize time-dependent PDEs

Space-time discretizations

From a space-time variational formulation

• Space-time DPG/LS methods

Method of discretization in time

FD in time + sequence of variational problems in space

• BE in time + DPG/LS in space

Method of Lines

Discretization in space + system of ODEs

• Bubnov-Galerkin in space + Exponential Integrators in time

Motivation

Main Focus: Discontinuous Petrov-Galerkin (DPG) method

In the context of Method of Lines

- Create a new time-marching scheme based on the DPG method
- Couple it with DPG semidiscretizations in space

Contributions:

- J. Muñoz-Matute, D. Pardo, and L. Demkowicz, Equivalence between the DPG method and the Exponential Integrators for linear parabolic problems, Journal of Computational Physics, 2021, vol. 429, pp. 110016.
- [2] J. Muñoz-Matute, D. Pardo, and L. Demkowicz, A DPG-based time-marching scheme for linear hyperbolic problems, Computer Methods in Applied Mechanics and Engineering, 2021, vol. 373, pp. 113539.
- [3] J. Muñoz-Matute, L. Demkowicz, and D. Pardo, Error representation of the time-marching DPG scheme, Computer Methods in Applied Mechanics and Engineering, 2022, vol. 391, pp. 114480.
- [4] J. Muñoz-Matute, L. Demkowicz, and N. Roberts, Combining DPG in space with DPG time-marching scheme for transient advection-reaction problems, Computer Methods in Applied Mechanics and Engineering, 2022, In press.

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1 Summary of the DPG time-marching scheme

2 Coupling with DPG semidiscretization in space

3 Computing exponential related functions

4 Current and Future work

System of ODEs

Let I = (0, T) with T > 0

$$\begin{cases} U'(t) + AU(t) = F(t), \ \forall t \in \overline{I} \\ U(0) = U_0 \end{cases}$$

where $A \in \mathbb{R}^{s \times s}$ and $U_0 \in \mathbb{R}^{s \times 1}$.

We define a mesh I_{τ} of I

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

where $I_k = (t_{k-1}, t_k)$, $\tau = t_k - t_{k-1}$, $\forall k = 1, ..., m$ and Γ_{τ} denotes the mesh skeleton in time.

Variational formulation

Broken ultraweak variational formulation

Denoting by $\mathbb{U} := L^2(I, \mathbb{R}^s)$ and $\mathbb{V} := H^1(I_\tau, \mathbb{R}^s)$

$$\begin{cases} \text{Find } U \in \mathbb{U} \text{ and } \hat{U} = (\hat{U}^1, \dots, \hat{U}^m) \in \mathbb{R}^{s \times m} \text{ s.t.} \\ B_\tau(U, V) + \langle \hat{U}, V \rangle_{\Gamma_\tau} = \int_I (F(t), V) dt + U_0 V(0), \ \forall V \in \mathbb{V} \end{cases}$$

where

$$B_ au(U,V)+\langle\hat{U},V
angle_{\Gamma_ au}:=\sum_{k=1}^m\int_{I_k}(U,-V'+A^TV)dt-(\hat{U}^k,[V]_k).$$

Here, (\cdot, \cdot) denotes the usual dot product in \mathbb{R}^s and $[V]_k = V(t_k^+) - V(t_k^-), \ \forall k = 1, \dots, m-1 \text{ and } [V]_m = -V(t_m^-).$

Optimal test functions corresponding to fields

Given
$$\delta U \in \mathbb{U}$$
 find $V_{\delta U} \in \mathbb{V}$ s.t
 $(V_{\delta U}, \delta V)_{\mathbb{V}} = B_{\tau}(\delta U, \delta V), \ \forall \delta V \in \mathbb{V}$

Optimal test functions corresponding to traces

$$\begin{cases} \text{Given } \delta \hat{U} \in \mathbb{R}^{s \times m} \text{ find } V_{\delta \hat{U}} \in \mathbb{V} \text{ s.t} \\ (V_{\delta \hat{U}}, \delta V)_{\mathbb{V}} = \langle \delta \hat{U}, \delta V \rangle_{\Gamma_h}, \ \forall \delta V \in \mathbb{V} \end{cases}$$

where the inner product is

$$||V||_{\mathbb{V}}^2 = \sum_{k=1}^m ||-V' + A^T V||_{I_k}^2 + |V(t_k^-)|^2,$$

where $|| \cdot ||_{I_k}$ denotes the L^2 -norm over each time interval I_k .

Optimal test functions for piecewise polynomials

Approximation of the field variables

$$U(t)_{|_{I_k}} \approx U_{\tau}^k(t) := \sum_{l=0}^q U_{\tau,l}^k \left(\frac{t-t_{k-1}}{\tau}\right)^l, \; \forall k = 1, \dots, m,$$

The optimal test functions are defined recursively at each time interval $\forall k = 1, ..., m$ as

$$\begin{cases} \hat{V}^{k}(A^{T},t) = e^{A^{T}(t-t_{k})} \\ V_{r}^{k}(A^{T},t) = (A^{T})^{-1} \left(\left(\frac{t-t_{k-1}}{\tau} \right)^{r} I_{s} + \frac{r}{\tau} V_{r-1}^{k}(A^{T},t) - \hat{V}^{k}(A^{T},t) \right) \\ \forall r = 0, \dots, q \end{cases}$$

$$\begin{cases} \hat{U}^{k} = \hat{V}(A, t_{k-1})\hat{U}^{k-1} + \int_{I_{k}}\hat{V}(A, t)F(t)dt \\ \sum_{l=0}^{q} U_{\tau,l}^{k} \int_{I_{k}} \left(\frac{t - t_{k-1}}{\tau}\right)^{l+r} dt = V_{r}^{k}(A, t_{k-1})\hat{U}^{k-1} + \int_{I_{k}} V_{r}^{k}(A, t)F(t)dt \end{cases}$$

 $\forall r = 0, \ldots, q \text{ and } \hat{U}^0 = U_0.$



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$$\forall r = 0, \ldots, q \text{ and } \hat{U}^0 = U_0.$$



Example: 1D+time heat equation

1D+time heat equation

Let
$$I = (0, T)$$
 with $T > 0$ and $\Omega = (0, 1)$

$$\begin{cases} u_t(x,t) - u_{xx}(x,t) = f(x,t), & \text{in } \Omega \times I \\ u(0,t) = u(1,t) = 0, & \text{in } I \\ u(x,0) = u_0(x), & \text{in } \Omega \end{cases}$$

Bubnov-Galerkin method in space

$$\begin{cases} (u_t(t), v) + (u_x(t), v_x) = (f(t), v), & \forall v \in H_0^1(\Omega) \\ (u(0), w) = (u_0, w), & \forall w \in L^2(\Omega) \end{cases}$$

<u>Approximation</u>: $\mathcal{V}_h = \operatorname{span}\{\phi_j(x)\} \subset H^1_0(\Omega), u_h(x,t) = \sum_{j=1}^s u_{h,j}(t)\phi_j(x)$

Square system of ODEs: $A = M^{-1}K$

$$\begin{cases} MU'(t) + KU(t) = F(t), \ \forall t \in I \\ M_0 U(0) = U_0 \end{cases}$$

Example: 1D+time heat equation



Approximated solution for q = 0, 1, 2.

1D+time advection-reaction equation

Let I = (0, T) with T > 0 and $\Omega = (0, 1)$

$$\begin{cases} u_t(x,t) + bu_x(x,t) + cu(x,t) = f(x,t), & \text{in } \Omega \times I \\ u(0,t) = g(t), & \text{in } I \\ u(x,0) = u_0(x), & \text{in } \Omega \end{cases}$$

where b and c are positive constants.

We define a mesh Ω_h of Ω

$$0 = x_0 < x_1 < \ldots < x_{n-1} < x_n = 1,$$

where $\Omega_i = (x_{i-1}, x_i)$, $h = x_i - x_{i-1}$, $\forall i = 1, ..., n$ and Γ_h denotes the mesh skeleton in space.

- Petrov-Galerkin method
- Discontinuous Petrov-Galerkin method
- Practical Discontinuous Petrov-Galerkin method

Test space:
$$H^1_+(\Omega) := \{ v \in H^1(\Omega) \mid v(1) = 0 \}.$$

PG formulation

Find
$$u \in C^1(\overline{I}; L^2(\Omega))$$
 s.t. $\forall t \in \overline{I}$
 $(u_t(t), v) + \mathfrak{b}(u(t), v) = \tilde{f}(t, v), \quad \forall v \in H^1_+(\Omega)$
 $(u(0), w) = (u_0, w), \quad \forall w \in L^2(\Omega)$

where

$$b(u(t), v) := (u(t), -bv_x + cv)$$

$$\tilde{f}(t, v) := (f(t), v) + g(t)bv(0)$$

Petrov-Galerkin discretization

Discrete spaces: $s := \dim(\mathcal{U}_h) = \dim(\mathcal{V}_h)$

$$\mathcal{U}_h := \mathcal{P}^p(\Omega_h), \ \mathcal{V}_h := \mathcal{P}^{p+1}(\Omega_h) \cap H^1_+(\Omega)$$

PG discretization

Find
$$u_h \in C^1(\overline{I}; \mathcal{U}_h)$$
 s.t. $\forall t \in \overline{I}$
 $(u_{h,t}(t), v_h) + \mathfrak{b}(u_h(t), v_h) = \tilde{f}(t, v_h) \qquad \forall v \in \mathcal{V}_h,$
 $(u_h(0), w_h) = (u_0, w_h), \quad \forall w_h \in \mathcal{U}_h$

Square system of ODEs: $A = M^{-1}K$

$$\begin{cases} MU'(t) + KU(t) = \tilde{F}(t), \ \forall t \in \bar{I} \\ M_0 U(0) = \tilde{U}_0 \end{cases}$$

- Optimal choice of spaces for u' = f (symmetric *K*).
- Rectangular system in higher dimensions.

DPG formulation

Trial and test spaces: $\mathcal{U} := L^2(\Omega)$ and $\mathcal{V} := H^1(\Omega_h)$

DPG formulation

$$\begin{array}{l} \text{Find } u \in C^1(\bar{I};\mathcal{U}) \text{ and } \bar{u} = (\bar{u}^1, \dots, \bar{u}^n) \in C(\bar{I}) \text{ s.t. } \forall t \in \bar{I} \\ (u_t(t), v) + \mathfrak{b}_h(u(t), v) + \langle \bar{u}(t), v \rangle_{\Gamma_h} = \tilde{f}(t, v), & \forall v \in \mathcal{V} \\ (u(0), w) = (u_0, w), & \forall w \in \mathcal{U} \end{array}$$

We define time-dependent interface variables

$$\bar{u}^i(t) := u(x_i, t), \ \forall i = 1, \dots, n,$$

and the bilinear form is

$$\mathfrak{b}_h(u(t),v)+\langle ar{u}(t),v
angle_{\Gamma_h}:=\sum_{i=1}^n(u(t),-bv_x+cv)_{\Omega_i}-\sum_{i=1}^nar{u}^i(t)b[v]_i,$$

where $[v]_i = v(x_i^+) - v(x_i^-), \ \forall i = 1, \dots, n-1 \text{ and } [v]_n = -v(x_n^-).$

DPG discretization



DPG discretization

Selecting

$$\mathcal{U}_h := \mathcal{P}^p(\Omega_h), \ \mathcal{V}_h := \mathcal{P}^{p+\Delta p}(\Omega_h),$$

with $\Delta p \geq 1$, we obtain a rectangular system

$$\begin{cases} MU'(t) + KU(t) + R\bar{u}(t) = \tilde{F}(t), \ \forall t \in \bar{I} \\ M_0 U(0) = \tilde{U}_0 \end{cases}$$

Optimal testing

$$\begin{cases} \text{Given } \delta u \in \mathcal{U} \text{ find } v_{\delta u} \in \mathcal{V} \text{ s.t} \\ (v_{\delta u}, \delta v)_{\mathcal{V}} = \mathfrak{b}_h(\delta u, \delta v), \ \forall \delta v \in \mathcal{V}, \end{cases} \\ \begin{cases} \text{Given } \delta \bar{u} \in \mathbb{R}^n \text{ find } v_{\delta \bar{u}} \in \mathcal{V} \text{ s.t} \\ (v_{\delta \bar{u}}, \delta v)_{\mathcal{V}} = \langle \delta \bar{u}, \delta v \rangle_{\Gamma_h}, \ \forall \delta v \in \mathcal{V}. \end{cases}$$

<u>Discretization</u>:For any $\delta u_h \in \mathcal{U}_h$ and $\delta \bar{u} \in \mathbb{R}^n$ we have

$$v_{\delta u_h} = G^{-1} K \delta u_h, \quad v_{\delta \overline{u}} = G^{-1} R \delta \overline{u}.$$

DPG discretization

We obtain the following square system of ODEs

$$\begin{cases} K^{T}G^{-1}MU'(t) + K^{T}G^{-1}KU(t) + K^{T}G^{-1}R\bar{u}(t) = K^{T}G^{-1}\tilde{F}(t), \ \forall t \in \bar{I} \\ R^{T}G^{-1}MU'(t) + R^{T}G^{-1}KU(t) + R^{T}G^{-1}R\bar{u}(t) = R^{T}G^{-1}\tilde{F}(t) \\ M_{0}U(0) = \tilde{U}_{0} \end{cases}$$

Eliminating the interface variables

$$\begin{cases} K^T S_1 M U'(t) + K^T S_1 K U(t) = K^T S_1 \tilde{F}(t), \ \forall t \in \overline{I} \\ M_0 U(0) = \tilde{U}_0 \end{cases}$$

where

$$S_1 = G^{-1} - G^{-1}R(R^T G^{-1}R)^{-1}R^T G^{-1}$$

and the matrix A of the system is

$$A = (K^T S_1 M)^{-1} K^T S_1 K.$$

Matrices K, M and G are block diagonal but R is not $\Longrightarrow K^T S_1 M$ is dense Non practical!

We maintain the optimal test function $v_{\delta u}$ for the fields and we introduce

$$\begin{cases} \text{Given } \delta \bar{u} \in \mathbb{R}^n \text{ find } v_{\delta \bar{u}} \in \mathcal{V} \text{ and } u \in \mathcal{U} \text{ s.t} \\ (v_{\delta \bar{u}}, \delta v)_{\mathcal{V}} - \mathfrak{b}_h(u, \delta v) = \langle \delta \bar{u}, \delta v \rangle_{\Gamma_h}, \ \forall \delta v \in \mathcal{V} \\ (\delta u, v_{\delta \bar{u}}) = 0, \qquad \forall \delta u \in \mathcal{U} \end{cases}$$

Discretizing we obtain $v_{\delta \bar{u}} = S_2^T R \delta \bar{u}$ where

$$S_2 = G^{-1} - G^{-1}M(K^TG^{-1}M)^{-1}K^TG^{-1}$$

which leads to the following system of ODEs

$$\begin{cases} K^{T}G^{-1}MU'(t) + K^{T}G^{-1}KU(t) + K^{T}G^{-1}R\bar{u}(t) = K^{T}G^{-1}\tilde{F}(t), \ \forall t \in \bar{I}, \\ R^{T}S_{2}KU(t) + R^{T}S_{2}R\bar{u}(t) = R^{T}S_{2}\tilde{F}(t), \\ M_{0}U(0) = \tilde{U}_{0}, \end{cases}$$
(2.1)

Eliminating the interface variables we obtain the final system

$$\begin{cases} K^T G^{-1} M U'(t) + K^T S_3 K U(t) = K^T S_3 \tilde{F}(t), \ \forall t \in \overline{I} \\ M_0 U(0) = \tilde{U}_0 \end{cases}$$

where

$$S_3 = G^{-1} - G^{-1}R(R^T S_2 R)^{-1}R^T S_2$$

and the matrix is

$$A = (K^T G^{-1} M)^{-1} K^T S_3 K$$

Here, the inversion of matrix $K^T G^{-1} M$ can be computed locally.

The method is consistent with steady-state solutions.

Adjoint graph norm

$$||v||_{\mathcal{V}}^2 = \sum_{i=1}^n ||v||_{\Omega_i}^2 + ||-bv_x + cv||_{\Omega_i}^2$$

Localizable adjoint norm

$$||v||_{\mathcal{V}}^2 = \sum_{i=1}^n ||-bv_x + cv||_{\Omega_i}^2 + b|v(x_i^-)|^2$$

where $|| \cdot ||_{\Omega_i}$ denotes the L^2 -norm over each element Ω_i .

For pure advection (c = 0), the adjoint graph norm leads a singular $K^T G^{-1} M$ matrix.

Numerical results

Some observations:

- No difference between employing practical and classical DPG methods and adjoint or adjoint graph norm.
- For pure convection problems the three discretizations in space deliver the same solution.
- For convection-reaction problems, the PG discretization is suboptimal. Error for the fields:

$$\mathcal{E} := \left(\int_{I} \left|\left|u(x,t) - u_{\tau h}(x,t)\right|\right|_{L^{2}(\Omega)}^{2} dt\right)^{1/2}$$

Error for the traces:

$$\hat{\mathcal{E}}_{1} := \left(\sum_{k=1}^{m} ||u(x,t_{k}) - \hat{u}_{h}^{k}(x)||_{L^{2}(\Omega)}^{2}\right)^{1/2}$$
$$\hat{\mathcal{E}}_{2} := \max_{1 \le k \le m} ||u(x,t_{k}) - \hat{u}_{h}^{k}(x)||_{L^{2}(\Omega)}$$

Pure advection: smooth solution



Approximation of fields with $p = \underset{24/38}{0} 1$ (rows) and q = 0, 1 (columns).

Pure convection: smooth solution



Approximation of traces with p = 0, 1 (rows) and q = 0, 1 (columns).

Pure advection: smooth solution



Optimal convergence rates both time and space: $\mathcal{O}(\tau^{q+1})$ and $\mathcal{O}(h^{p+1})$

Pure advection: smooth solution



Solid lines refer to error $\hat{\mathcal{E}}_1$ and dashed lines to error $\hat{\mathcal{E}}_2$.

Rates in space for both $\hat{\mathcal{E}}_1$ and $\hat{\mathcal{E}}_2$: $\mathcal{O}(h^{p+1})$ Rate in time for $\hat{\mathcal{E}}_2$: $\mathcal{O}(\tau^{q+1})$ and for $\hat{\mathcal{E}}_1$: $\mathcal{O}(\tau^{q+1/2})$

Large reaction term



PG method in space (top row) and DPG method (bottom row) for p = 0, 1, 2 and $\Delta p = 2$. Reaction term $c = 10^4$.

Large reaction term



Large reaction term



Transport problem: Continuous non-smooth solution



Approximation of fields (left) and traces (center) for p = q = 1.



Transport problem: Discontinuous solution (traces)



Snapshots a discontinuous solution with q = 0 and p = 2. Trace variables for a fine grid in time and different mesh sizes space.

Transport problem: Discontinuous solution (fields)



Snapshots a discontinuous solution with q = 0 and p = 2. First row: Field variables for a fine grid in time and different mesh sizes in space. Second row: Field variables for a fine mesh in space and different time step sizes.

Exponential quadrature rule

Time-marching scheme: $\forall k = 1, \dots, m$ and $\forall r = 0, \dots, q$

$$\begin{cases} \hat{U}^{k} = \hat{V}(A, t_{k-1})\hat{U}^{k-1} + \int_{I_{k}}\hat{V}(A, t)F(t)dt\\ \sum_{l=0}^{q} U_{\tau,l}^{k} \int_{I_{k}} \left(\frac{t - t_{k-1}}{\tau}\right)^{l+r} dt = V_{r}^{k}(A, t_{k-1})\hat{U}^{k-1} + \int_{I_{k}} V_{r}^{k}(A, t)F(t)dt \end{cases}$$

the optimal test functions can be expressed in terms of the so-called φ -functions

$$\begin{cases} \varphi_0(z) = e^z, \\ \varphi_q(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{q-1}}{(q-1)!} d\theta, \ \forall q \ge 1, \end{cases}$$

Lowest order method (r = 0)

$$\begin{cases} \hat{U}^{k} = \hat{U}^{k-1} + \tau \varphi_{1}(-\tau A)(F(t_{k-1}) - A\hat{U}^{k-1}) \\ U^{k}_{\tau,0} = \varphi_{1}(-\tau A)\hat{U}^{k-1} + \tau \varphi_{2}(-\tau A)F(t_{k-1}) \end{cases}$$

Approximating the action φ -functions

Theorem

Let
$$A \in \mathbb{R}^{s \times s}$$
, $W = [w_1, \ldots, w_q] \in \mathbb{R}^{s \times q}$, and

$$\widetilde{A} = \begin{bmatrix} A & W \\ 0 & J \end{bmatrix} \in \mathbb{R}^{(s+q) \times (s+q)}, \ J = \begin{bmatrix} 0 & I_{q-1} \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{q \times q};$$

it holds that
$$e^{\tilde{A}}b_j(1:s) = \sum_{l=1}^{J} \varphi_l(A)w_{j-l+1}, \quad \forall j = 1, \dots, q,$$

b_j being the j-vector in the canonical basis in \mathbb{R}^s .

Scaling and squaring algorithm + truncated Taylor series

$$e^{\tilde{A}}b_j \approx \left(T_m\left(\frac{1}{\sigma}\tilde{A}\right)\right)^{\sigma}b_j,$$

The values of *m* and σ are selected based on the sequence of norms: $\|\tilde{A}^k\|_1^{1/k}$.

 A. H. Al-Mohy and N. J. Higham Computing the action of the matrix exponential, with an application to exponential integrators, SIAM Journal on Scientific Computing, 33(2):488-511, 2011. We have $s := \dim(\mathcal{U}_h)$ and $r := \dim(\mathcal{V}_h)$, where $r \gg s$

 $M, K \in \mathbb{R}^{r \times s}, \ G \in \mathbb{R}^{r \times r}, \ R \in \mathbb{R}^{r \times n},$

n being the number of interface variables in space.

Then, we can rewrite the final matrix of the system as

$$A = \underbrace{(K^{T}G^{-1}M)^{-1}K^{T}G^{-1}K}_{A_{1}} - \underbrace{(K^{T}G^{-1}M)^{-1}K^{T}G^{-1}R}_{A_{2}}\underbrace{(R^{T}S_{2}R)^{-1}}_{A_{3}}\underbrace{R^{T}S_{2}K}_{A_{4}},$$

where

• $A_1 \in \mathbb{R}^{s \times s}$ and $S_2 \in \mathbb{R}^{r \times r}$ are block diagonal.

- $A_2 \in \mathbb{R}^{s \times n}$ and $A_4 \in \mathbb{R}^{n \times s}$ are sparse and thin.
- $A_3 \in \mathbb{R}^{n \times n}$ is dense but small.

Current work

• Speed-up the computation of φ -functions for matrices with Kronecker sum structure.



J. Muñoz-Matute, D. Pardo, and V. M. Calo,

Exploiting the Kronecker product structure of φ -functions with applications to exponential time integrators,

International Journal for Numerical Methods in Engineering, 2022, pp.1-20.

M. Croci and J. Muñoz-Matute,

Exploiting Kronecker structure in exponential integrators: fast approximation of the action of φ -functions via quadrature, To be submitted soon.

• Multistage version of the DPG scheme for semi-linear problems.



J. Muñoz-Matute, D. Pardo, and L. Demkowicz,

Multistage DPG time-marching scheme for semi-linear problems, In preparation.

• MinRes methods in the dual norm employing neural networks.

C. Uriarte, D. Pardo, I. Muga, and J. Muñoz-Matute, A deep double Ritz method for solving partial differential equations, To be submitted soon.

Possible research lines:

- To extend the implementation of the presented DPG semidiscretization in space together with DPG time-marching scheme to higher dimensions.
- (Goal-oriented) adaptivity in space together with adaptivity in time.
- Apply the Kronecker algorithm for 3D+time phase-field models with IGA (GPUs/parallelization).
- Develop an adaptive strategy in time for the Multistage DPG method.
- To employ deep neural networks to approximate the action of the exponential-related functions.