Efficient Numerical Methods for Weak Solutions of Partial Differential Equations

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Outline of Talk

1. Conventional Numerical Methods
    - Weak Galerkin (WG) Finite Element Methods
    - Primal-Dual Weak Galerkin (PDWG) Finite Element Methods (FEM)
2. Deep Learning (DL)
    - Friedrichs Learning: Weak Solutions of PDEs

1. **Model Problem:** Find u satisfying $u|_{\partial\Omega} = 0$, such that

$$-\Delta u = f, \qquad \text{in} \quad \Omega.$$

2. **Weak Form:** Find $u \in H_0^1(\Omega)$ such that

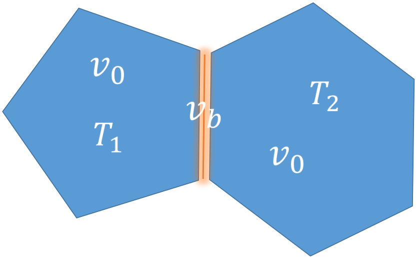
$$(\nabla u, \nabla v) = (f, v), \qquad \forall v \in H_0^1(\Omega).$$

Weak Galerkin Finite Element Methods

$\mathcal{T}_h$: **polygonal/polytopal partition** of the domain Ω, shape regular

Weak Functions

A **weak function** on the finite element partition $\mathcal{T}_h$ refers to a generalized function $v = \{v_0, v_b\}$ such that $v_0 \in L^2(T)$ and $v_b \in L^2(\partial T)$ for any $T \in \mathcal{T}_h$ with single value v_b on shared edges.



Weak Gradient and Discrete Weak Gradient

The **weak gradient** of $v = \{v_0, v_b\}$ is defined as a bounded linear functional $\nabla_w v$ in $[H^1(T)]^2$ whose action on each $q \in [H^1(T)]^2$ is given by

$$\langle \nabla_w v, q \rangle_K := -\int_K v_0 \nabla \cdot q dK + \int_{\partial K} v_b q \cdot \mathbf{n} ds.$$

For computational purpose, the weak gradient needs to be approximated

Discrete weak gradient

Find $\nabla_{w,r} v \in [P_r(T)]^2$ such that

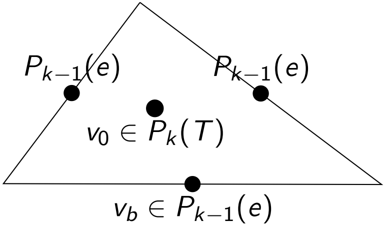
$$\int_K \nabla_{w,r} v \cdot q dK = -\int_K v_0 \nabla \cdot q dK + \int_{\partial K} v_b q \cdot \mathbf{n} ds,$$

for all $q \in [P_r(T)]^2$.

Weak Finite Element Spaces

- On each $T \in \mathcal{T}_h$, the local finite element space is

$$V_k(T) := \{v = \{v_0, v_b\} : \ v_0 \in P_k(T), v_b \in P_{k-1}(\partial T)\}.$$



- Global weak finite element space:

$$V_h := \{v = \{v_0, v_b\} : \ \{v_0, v_b\}|_T \in V_k(T), \forall T \in \mathcal{T}_h\}.$$

- Weak finite element space with vanishing boundary value:

$$V_h^0 := \{v = \{v_0, v_b\} \in V_h, v_b|_{\partial\Omega} = 0\}.$$

Weak Galerkin Finite Element Formulation

WG-FEM

Find $u_h = \{u_0, u_b\} \in V_h^0$ such that

$$(\nabla_w u_h,\ \nabla_w v) + s(u_h, v) = (f, v_0), \qquad \forall v = \{v_0, v_b\} \in V_h^0,$$

where

1. $\nabla_w v \in [P_{k-1}(T)]^d$ is computed locally on each element.
2. $s(\cdot, \cdot)$ is a stabilizer enforcing a weak continuity.

Stabilizer $s(\cdot,\cdot)$

- Commonly used stabilizer:

$$s(w,v)=\rho\sum_{T\in\mathcal{T}_h} h_T^{-1}\langle Q_b w_0 - w_b, Q_b v_0 - v_b\rangle_{\partial T},$$

where Q_b is the L^2 projection onto $P_{k-1}(e), e\subset\partial T$, and $\rho>0$ is a parameter of free-choice.

- Discrete and computation-friendly stabilizer:

$$s(w,v)=\rho\sum_{T\in\mathcal{T}_h}\sum_{x_j\in\partial T}(w_0-w_b)(x_j)\,(v_0-v_b)(x_j),$$

where $\{x_j\}$ is a set of carefully chosen (nodal) points on ∂T.

An Abstract Framework

Abstract Problem

Find $u \in V$ such that

$$a(u, v) = f(v), \qquad \forall v \in V.$$

Assume

- V_h: finite dimensional spaces that approximate V
- $a_h(\cdot,\cdot)$: bilinear forms on $V_h \times V_h$ that approximate $a(\cdot,\cdot)$
- f_h: linear functionals on V_h that approximate f
- $s(\cdot,\cdot)$: stabilizers that provide necessary "smoothness"

Abstract WG

Find $u_h \in V_h$ such that

$$a_h(u_h, v) + s(u_h, v) = f_h(v), \quad \forall\ v \in V_h.$$

PDWG for PDEs in Non-Divergence Form

Model Problem: Find u satisfying $u|_{\partial\Omega} = 0$, such that

$$\sum_{i,j=1}^{d} a_{ij}\partial_{ij}^2 u = f, \quad \text{in } \Omega.$$

Assumptions:

- $a(x) = (a_{ij}(x))_{d\times d} \in [L^\infty(\Omega)]^{d\times d}$
- $a(x)$ is symmetric and uniformly positive definite in Ω

Theorem

Assume $\Omega \subset \mathbb{R}^d$ is a bounded convex domain, $a(x) \in [L^\infty(\Omega)]_{d\times d}$ is symmetric and uniformly positive definite in Ω, and the Cordès condition is satisfied. For any given $f \in L^2(\Omega)$, there exists a unique strong solution $u \in H^2(\Omega) \cap H_0^1(\Omega)$ satisfying

$$\|u\|_2 \leq C\|f\|_0.$$

- **Cordès condition:** There exists an $\varepsilon \in (0, 1]$ such that

$$\frac{\sum_{i,j=1}^d a_{ij}^2}{(\sum_{i=1}^d a_{ii})^2} \leq \frac{1}{d-1+\varepsilon} \qquad \text{in } \Omega.$$

Variational Equation

Variational Equation: Find $u \in X = H^2(\Omega) \cap H_0^1(\Omega)$ such that

$$b(u, w) = (f, w) \qquad \forall w \in Y = L^2(\Omega).$$

- $b(u, w) = (\sum_{i,j=1}^{d} a_{ij} \partial_{ij}^2 u, w)$
- $b(\cdot, \cdot)$ satisfies the **inf-sup** condition

$$\sup_{v \in X, v \neq 0} \frac{b(v, \sigma)}{\|v\|_X} \geq \Lambda \|\sigma\|_Y, \forall \sigma \in Y.$$

Discrete Weak Second Order Partial Derivative

$$W(T) = \{v = \{v_0, v_b, \mathbf{v}_g\} : v_0 \in L^2(T), v_b \in L^2(\partial T), \mathbf{v}_g \in [L^2(\partial T)]^d\}.$$

Weak Second Order Partial Derivative

The **weak second order partial derivative** of $v \in W(T)$ is defined as a bounded linear functional $\partial^2_{ij,w} v$ on $H^2(T)$ so that its action on each $\varphi \in H^2(T)$ is given by

$$\langle \partial^2_{ij,w} v, \varphi \rangle_K := (v_0, \partial^2_{ji}\varphi)_K - \langle v_b n_i, \partial_j \varphi \rangle_{\partial K} + \langle v_{gi}, \varphi n_j \rangle_{\partial K}.$$

Discrete Weak Second Order Partial Derivative

A **discrete weak second order partial derivative** of $v \in W(T)$, denoted by $\partial^2_{ij,w,r,K} v$, is defined as the unique polynomial satisfying

$$(\partial^2_{ij,w,r,K} v, \varphi)_K = (v_0, \partial^2_{ji}\varphi)_K - \langle v_b n_i, \partial_j \varphi \rangle_{\partial K} + \langle v_{gi}, \varphi n_j \rangle_{\partial K}, \forall \varphi \in P_r(T).$$

Naive WG-FEM

Find $u_h = \{u_0, u_b, \mathbf{u}_g\}$ such that

$$b_h(u_h, \sigma) = (f, \sigma), \qquad \forall \sigma,$$

where $b_h(u_h, \sigma) := \sum_{T \in \mathcal{T}_h} \sum_{i,j=1}^{d} (a_{ij} \partial^2_{ij,w} u_h, \sigma)_T$.

PDWG as constrained optimization

Find $u_h = \{u_0, u_b, \mathbf{u}_g\} \in V_h^0$ such that

$$u_h = \underset{v\in V_h^0, b_h(v,\sigma)=(f,\sigma), \forall \sigma \in W_h}{\arg\min} \frac{1}{2} s_h(v, v).$$

- **Stabilizer** that enforces weak continuity:

$$s_h(v, v) = \sum_{T\in\mathcal{T}_h} h_T^{-3} \langle v_0 - v_b, v_0 - v_b \rangle_{\partial T} + h_T^{-1} \langle \nabla v_0 - \mathbf{v}_g, \nabla v_0 - \mathbf{v}_g \rangle_{\partial T}$$

PDWG - FEM in Euler-Lagrange Form

PDWG Algorithm

Find $(u_h;\lambda_h) \in V_h^0 \times W_h$ satisfying

$$
\begin{aligned}
s_h(u_h, v) + b_h(v, \lambda_h) &= 0, && \forall v \in V_h^0,\\
b_h(u_h, \sigma) &= (f, \sigma), && \forall \sigma \in W_h.
\end{aligned}
$$

- Weak finite element space V_h consisting of $P_k(T)/P_k(e)/[P_{k-1}(e)]^d$
- W_h : **Lagrange multiplier** finite element space of $P_{k-2}(T)$ or $P_{k-1}(T)$
- Primal equation: $b_h(u_h, \sigma) = (f, \sigma)$
- Dual equation: $b_h(v, \lambda_h) = 0$
- Linker: the stabilizer $s_h(u_h, v)$

Inf-Sup Condition

Lemma

Assume that the coefficient matrix $a = \{a_{ij}\}_{d\times d}$ is uniformly piecewise continuous in Ω. For any $\sigma \in W_h$, there exists $v_\sigma \in V_h^0$ satisfying

$$
\begin{aligned}
b_h(v_\sigma, \sigma) &\geq \frac{1}{2}\|\sigma\|_0^2, \\
\|v_\sigma\|_{2,h}^2 &\leq C\|\sigma\|_0^2.
\end{aligned}
$$

Here,

$$
\|v\|_{2,h}^2 = \sum_{T\in\mathcal{T}_h} \| \sum_{i,j=1}^{d} \mathcal{Q}_h(a_{ij}\partial_{ij}^2 v_0)\|_T^2 + s_h(v, v).
$$

Error Estimates

Theorem

Assume that the coefficient functions a_{ij} *are uniformly piecewise continuous in* Ω. *Let* u *and* $(u_h; \lambda_h) \in V_h^0 \times W_h$ *be the exact solution and PDWG solution. There exists a constant* C *such that*

$$\|u_h - Q_h u\|_{2,h} + \|\lambda_h - \mathcal{Q}_h \lambda\|_0 \leq C h^{k-1} \|u\|_{k+1}.$$

Numerical Tests

- Exact solution $u = sin(x_1)sin(x_2)$
- $\Omega = (-1, 1)^2$
- $a_{11} = 1 + |x_1|$, $a_{12} = a_{21} = 0.5|x_1 x_2|^{\frac{1}{3}}$, $a_{22} = 1 + |x_2|$

Table: numerical error and convergence order (λ_h is piecewise linear)

$2/h$	$\|e_0\|_0$	order	$\|\mathbf{e}_g\|_{L^2}$	order	$\|\lambda_h\|_0$	order
1	0.177	-	1.25	-	0.00390	-
2	0.0357	2.30	0.486	1.36	0.00820	-1.07
4	0.00360	3.31	0.130	1.90	0.00324	1.34
8	2.78e-004	3.70	0.0318	2.03	0.00151	1.10
16	2.02e-005	3.78	0.00783	2.02	7.42e-004	1.03
32	2.37e-006	3.09	0.00194	2.01	3.68e-004	1.01

Numerical Tests

Table: numerical error and convergence order (λ_h is piecewise constant)

$2/h$	$\|e_0\|_0$	order	$\|\mathbf{e}_g\|_{L^2}$	order	$\|\lambda_h\|_0$	order
1	2.80e-006	-	1.76	-	2.10e-006	-
2	0.176	-16.0	0.676	1.38	0.0895	-15.4
4	0.0395	2.15	0.164	2.04	0.0518	0.790
8	0.00896	2.14	0.0386	2.08	0.0190	1.45
16	0.00217	2.05	0.00938	2.04	0.00685	1.47
32	5.37e -004	2.01	0.00231	2.02	0.00288	1.25

Numerical Tests

Consider

$$\sum_{i,j=1}^{2}(1+\delta_{ij})\frac{x_i}{|x_i|}\frac{x_j}{|x_j|}\partial_{ij}^2 u = f, \qquad \text{in} \quad \Omega = (-1,1)^2,$$

$$u = 0, \qquad \text{on} \quad \partial\Omega,$$

with the exact solution $u = (x_1 e^{1-|x_1|} - x_1)(x_2 e^{1-|x_2|} - x_2)$.

Table: Numerical error and convergence order (λ_h is piecewise linear).

$2/h$	$\|e_0\|_0$	order	$\|\mathbf{e}_g\|_{L^2}$	order	$\|\lambda_h\|_0$	order
1	0.0940	-	0.766	-	0.338	-
2	0.249	-1.40	1.35	-0.815	0.642	-0.927
4	0.106	1.23	0.538	1.32	1.28	-1.00
8	0.0306	1.80	0.137	1.97	0.537	1.26
16	0.00749	2.03	0.0327	2.07	0.212	1.34
32	0.00174	2.11	0.00785	2.06	0.0923	1.20

Numerical Tests

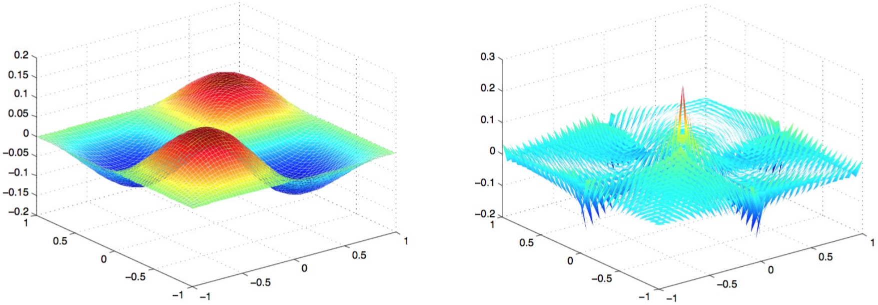


Figure: Figures for WG-solution u_0 and λ_h

Table: Numerical error and convergence order (λ_h is piecewise constant).

$2/h$	$\|e_0\|_0$	order	$\|\mathbf{e}_g\|_{L^2}$	order	$\|\lambda_h\|_0$	order
1	0.0393	-	0.672	-	0.137	-
2	0.0322	0.284	0.322	1.06	0.104	0.396
4	0.00750	2.10	0.0791	2.03	0.0532	0.963
8	0.00161	2.22	0.0180	2.13	0.0204	1.39
16	3.85e-004	2.07	0.00427	2.08	0.00818	1.32
32	9.52e-005	2.02	0.00104	2.04	0.00371	1.14

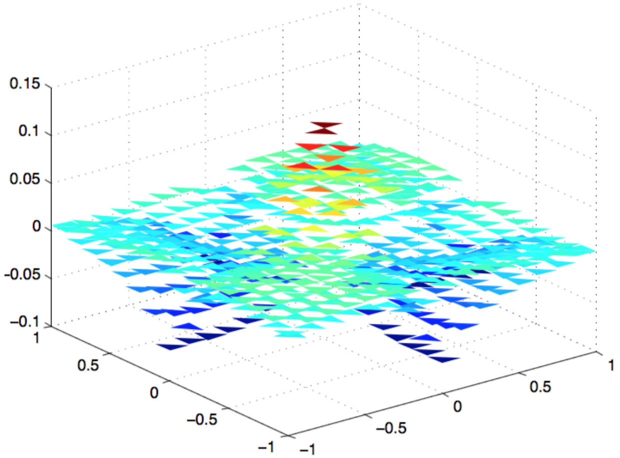


Figure: Figure for the Lagrange multiplier λ_h – an error indicator

Numerical Tests

$$\sum_{i,j=1}^{2}(\delta_{ij}+\frac{x_i x_j}{|x|^2})\partial_{ij}^2 u=(2\alpha^2-\alpha)|x|^{\alpha-2}, \qquad \text{in} \qquad (0,1)^2.$$

- Exact solution $u=|x|^{\alpha},\ \alpha>1$
- $\alpha=1.6$

Table: numerical error and convergence order(λ_h is piecewise linear)

$1/h$	$\|e_0\|_0$	order	$\|\mathbf{e}_g\|_{L^2}$	order	$\|\lambda_h\|_0$	order
1	0.020	-	0.315	-	0.304	-
2	0.00629	1.68	0.126	1.32	0.248	0.296
4	0.00174	1.86	0.0446	1.50	0.182	0.445
8	4.43e-004	1.97	0.0152	1.56	0.126	0.537
16	1.08e-004	2.03	0.00508	1.58	0.0846	0.570
32	2.60e-005	2.05	0.00169	1.59	0.0564	0.584

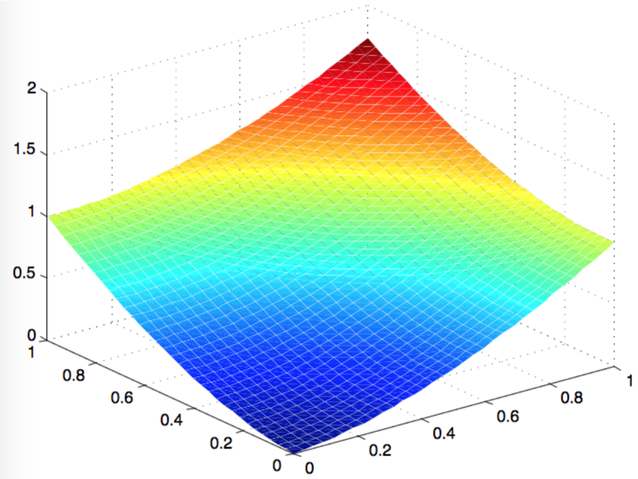


Figure: Figure for WG-solution u_0

Numerical Tests

Table: numerical error and convergence order (λ_h is piecewise constant)

$1/h$	$\|e_0\|_0$	order	$\|\mathbf{e}_g\|_{L^2}$	order	$\|\lambda_h\|_0$	order
1	0.00405	-	0.489	-	0.0623	-
2	0.00803	-0.988	0.177	1.46	0.0616	0.0156
4	0.00263	1.61	0.0616	1.53	0.0476	0.372
8	7.90e-004	1.74	0.0210	1.55	0.0327	0.544
16	2.20e-004	1.85	0.00705	1.57	0.0218	0.582
32	5.85e-005	1.91	0.00235	1.59	0.0145	0.593

An Abstract Problem

- Let V and W be two Hilbert spaces
- $b(\cdot, \cdot)$ is a bilinear form on $V \times W$
- The **inf-sup** condition of Babuska and Brezzi is satisfied.
- The spaces V and W have certain embedded "continuities", such as L^2, H^1, $H(div)$, $H(curl)$, H^2, or weighted-version of them.

Abstract Problem

Find $u \in V$ such that $b(u, w) = f(w)$ for all $w \in W$. Here f is a bounded linear functional on W.

An Abstract PDWG Formulation

PDWG-FEM

Find $u_h \in V_h$ and $\lambda_h \in W_h$ such that

$$\begin{aligned} s_1(u_h, v) - b_h(v, \lambda_h) &= 0, & \forall v \in V_h \\ s_2(\lambda_h, w) + b_h(u_h, w) &= f_h(w), & \forall\, w \in W_h. \end{aligned}$$

- $s_1(\cdot,\cdot)$: stabilizer/smoother in V_h
- $s_2(\cdot,\cdot)$: stabilizer/smoother in W_h

My work on PDWG methods includes

- second-order elliptic equations in non-divergence form
- Fokker-Planck type equations
- ill-posed elliptic Cauchy problem
- convection-diffusion equations arising from Poisson-Nernst-Planck modeling
- first-order transport problems
- second-order elliptic interface problem
- a simplified PDWG for the Fokker-Planck type equation
- a modified PDWG for the second order elliptic equation in non-divergence form

Numerical Experiments

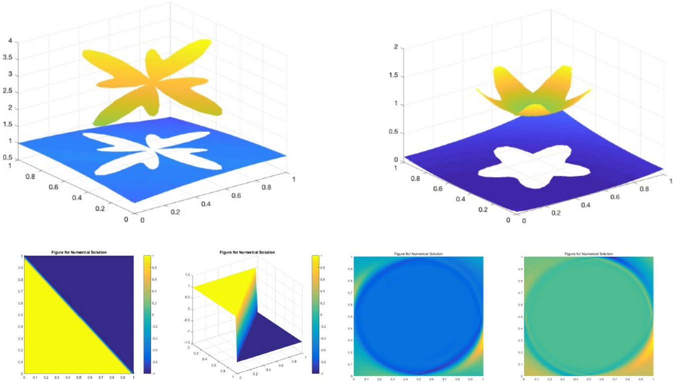


Figure: PDWG solutions.

Problem

$$\mathcal{D}(u) = f \quad \text{in } \Omega,$$
$$\mathcal{B}(u) = g \quad \text{on } \partial\Omega.$$

Physics Informed Neural Network (PINN):
A deep neural network (DNN) $\phi(\boldsymbol{x}; \boldsymbol{\theta}^*)$ is constructed to approximate the solution $u(\boldsymbol{x})$ via

$$\begin{aligned} \boldsymbol{\theta}^* &= \arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) \\ &:= \arg\min_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x}\in\Omega}\left[\left|\mathcal{D}\phi(\boldsymbol{x};\boldsymbol{\theta}) - f(\boldsymbol{x})\right|^2\right] + \\ &\quad \lambda \mathbb{E}_{\boldsymbol{x}\in\partial\Omega}\left[\left|\mathcal{B}\phi(\boldsymbol{x};\boldsymbol{\theta}) - g(\boldsymbol{x})\right|^2\right], \end{aligned}$$

where $\lambda > 0$.

Friedrichs Learning for Weak Solutions of PDEs

- **Original PDE problem**:

$$\text{find} \quad u \in V \quad \text{s.t.} \quad Tu = f \quad \text{for} \quad f \in L.$$

or equivalently,

$$(Tu, v)_L = (f, v)_L, \quad \forall\, v \in L.$$

- **New MinMax Formulation**:

$$\min_{u \in V} \max_{v \in V^*} \frac{|(u, \tilde{T} v)_L - (f, v)_L|}{\|\tilde{T} v\|_L}.$$

Friedrichs Learning for Weak Solutions of PDEs

Friedrichs Learning:

$$
\begin{aligned}
(\bar{\theta}_s, \bar{\theta}_t) &= \arg\min_{\theta_s}\max_{\theta_t} L(\phi_s(\boldsymbol{x};\theta_s), \phi_t(\boldsymbol{x};\theta_t)) \\
&= \arg\min_{\theta_s}\max_{\theta_t} \frac{|(\phi_s(\boldsymbol{x};\theta_s), \tilde{T}\phi_t(\boldsymbol{x};\theta_t))_\Omega - (f, \phi_t(\boldsymbol{x};\theta_t))_\Omega|}{\|\tilde{T}\phi_t(\boldsymbol{x};\theta_t)\|_\Omega},
\end{aligned}
$$

under the constraints

$$
\phi_s(\boldsymbol{x};\theta_s) \in V \text{ and } \phi_t(\boldsymbol{x};\theta_t) \in V^*.
$$

Parametrization:

- Tanh network ϕ_t for smooth test functions in V^*
- ReLU network $\phi_s \in H^1$ to approximate solutions in $V = L^2$
- Future: discontinuous networks for L^2 solutions

Model Problem:

$$\begin{aligned} \mu u + \boldsymbol{\beta} \cdot \nabla u =& f, \text{ in } \Omega = (-1,1)^2, \\ u =& g, \text{ on } \partial\Omega^- = \{\boldsymbol{x} \in \partial\Omega; \boldsymbol{\beta} \cdot \boldsymbol{n} < 0\}. \end{aligned}$$

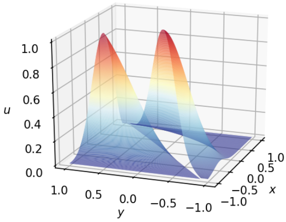
- assume there exists $\mu_0 > 0$ such that

$$\mu(\boldsymbol{x}) - \frac{1}{2}\nabla \cdot \boldsymbol{\beta}(\boldsymbol{x}) \geq \mu_0 > 0, \quad \text{a.e. in } \Omega$$

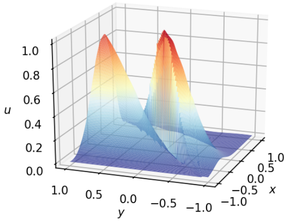
- $\boldsymbol{\beta} = (1, 9/10)^{\intercal}$, $\mu = 1$
- Exact solution:

$$u^* = \begin{cases} \sin(\pi(x+1)^2/4)\sin(\pi(y - \frac{9}{10}x)/2) & -1 \leq x \leq 1, \ \frac{9}{10}x < y \leq 1 \\ e^{-5(x^2 + (y - \frac{9}{10}x)^2)} & -1 \leq x \leq 1, \ -1 \leq y \leq \frac{9}{10}x \end{cases}$$

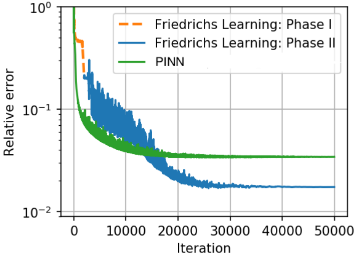
Numerical Tests: Advection-Reaction Equation



(a) Exact solution.



(b) NN solution.



(c) Comparison with PINN.

Numerical Tests: High-Dimensional Scalar Elliptic Equation

Model Problem:

$$-\nabla \cdot \left(a(\boldsymbol{x})\nabla u\right) = f \qquad \text{in } \Omega = (-1,1)^{15},$$
$$u = g \qquad \text{on } \partial\Omega,$$

- $a = 1 + |\boldsymbol{x}|^2$, $u^* = \sin(\frac{\pi x_1}{2})\cos(\frac{\pi x_2}{2})$

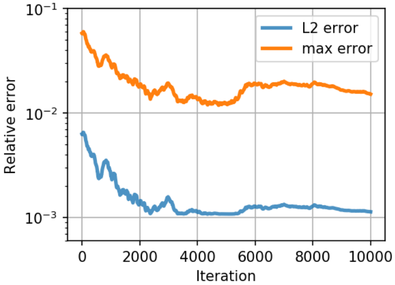
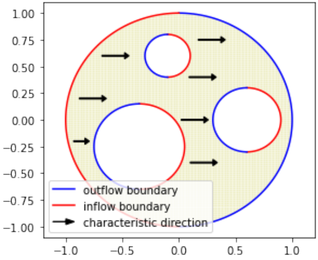


Figure: The relative error versus iteration.

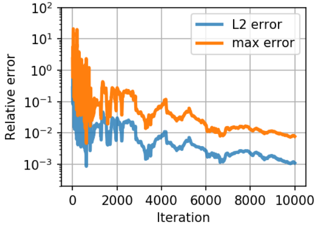
Numerical Tests: Linear Transport Equation

$$\begin{aligned} u_t + u_x =& 0, \text{ for } (t,x,y) \in \Omega, \\ u =& \sin(x+y), \text{for } t = 0, \end{aligned}$$

- $u^*(t,x,y) = \sin(x+y-t)$.



(a) Domain.



(b) The relative error versus iterations.

Thank you very much for your attention!

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