An Introduction to Over-Penalized Weak Galerkin Methods

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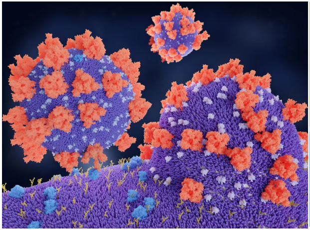
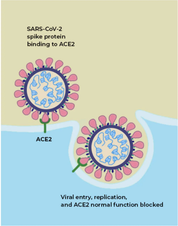
Outline

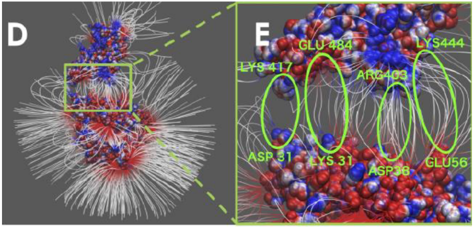
SARS-CoV-2 virus

Electrostatic binding between S-protein of the SARS-CoV-2 and ACE2 receptor on the surface of host cells.

- Identify strong binding sites between S-protein and ACE2
- Correlate binding affinity with COVID-19 variants
- Infectivity prediction
- Vaccine breakthrough
- Drug and antibody resistance

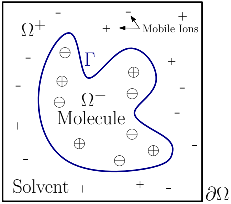






Classical (sharp interface) PB model

The Poisson-Boltzmann (PB) model is a mean field approach for calculating **electrostatic force and energy**. In the dimensionless form



$$\begin{cases} -\nabla\cdot(\epsilon\nabla u) + \chi_{\Omega_s}\kappa^2 \sinh u = \rho & \text{in} \quad \Omega; \\ u = u_b & \text{on} \quad \partial\Omega. \end{cases}$$

where u is the electrostatic potential, κ is the Debye-Hückel parameter, and ρ represents singular charge sources.

- $\Omega_m = \Omega^-$: inner solute (molecular) region;
- $\Omega_s = \Omega^+$: outer solvent region;
- $\Gamma = \partial\Omega_m \cap \partial\Omega_s$: solute-solvent interface or molecular surface.

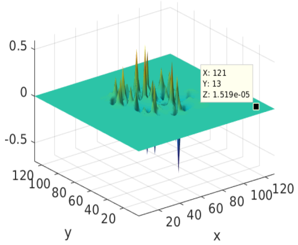
- **Two-dielectric PB model**: Using dielectric constants ϵ_m and ϵ_s, respectively, for the molecule and water, the dielectric function is

$$\epsilon = \epsilon_m \chi_{\Omega_m} + \epsilon_s \chi_{\Omega_s}.$$

Challenge: Singular partial charges of protein

- Each protein atom carries a point charge q_j located at the atom center $\mathbf{r_j}$. This gives rise to the singular source term of the PB model

$$\rho(\mathbf{r}) = \mathbf{4}\pi \frac{\mathbf{e_c^2}}{\mathbf{k_B T}} \sum_{\mathbf{j=1}}^{\mathbf{N_m}} \mathbf{q_j}\delta(\mathbf{r} - \mathbf{r_j}), \quad \text{in } \boldsymbol{\Omega},$$



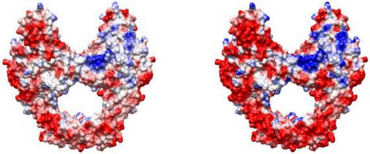
- Both ρ and potential u blow up at all atom centers!

- Traditional numerical approaches: (very inaccurate!)

1. **Trilinear** interpolation of charge to grid nodes in finite difference;
2. Evaluate through the trial function in Galerkin formulation.

$$\int C \sum_j q_j \delta(\mathbf{r} - \mathbf{r_j})\mathbf{v}(\mathbf{r}) = \mathbf{C} \sum_{\mathbf{j}} \mathbf{q_j v}(\mathbf{r_j}).$$

Poisson-Boltzmann models



Membrane Channel Charge Transport: Poisson-Nernst-Planck (PNP)+ Poisson-Boltzmann-Kohn-Sham (PBKS) models; Nonlinear Poisson-Boltzmann equation+interface conditions
The potential is decomposed into a singular part, a harmonic part, and a regular part.

- $\nabla \cdot \epsilon(r)\nabla\phi(r) - k\phi(r) = -4\pi\rho(r), \quad (\mathit{Linearization})$

Interface problems: The boundaries (complex surface) between regions of low and high dielectric are sharp.

Difficulties

(1) Low regularity: when a domain has reentrant corners/edges /interface corners, solution is usually not in $H^2(\Omega_i)$ $(i = 1, 2)$, instead, it is in a much larger spaces $H^{1+s}(\Omega_i)$ for some $0 < s < 1$; when the right-hand side is in $L^p(\Omega)$, the solution has a regularity estimate (see Book of Monique Dauge, 1988) in $W^{2,p}(\Omega_i)$ for some $p \in (1, 2)$.
(2) V_h: a finite element space consisting of discontinuous polynomials, i.e. $V_h \nsubseteq H_0^1(\Omega)$ and ∇v_h is not well defined for $v_h \in V_h$ in weak forms.
Existing solutions using discontinuous functions: IPDG; LDG; HDG; WG etc.

The existing numerical methods

- Delphi(Rocchia, Alexov, Honig, 01), CHARMM(Im, Beglov, Roux, 98), AMBER(Luo, David, Gilson, 02), APBS(Baker, Sept, Joseph, Holst, 01)
- LeVeque, Li (Immesed Interface Method, 94)
- Wei, Zhao, Geng (04, 09-15,22) (ADI, MIB, DG for NPB, diffuse interface, super Gaussian regularization)
- Cheng, Holst, Xu (FEM for NPB, 07)
- ......

Pioneer works on DG, WG

- Lions(68) (elliptic very rough Dirichlet boundary data)
- Babuška(73), Nitsche(71), Douglas & Dupont(76) and Baker(77) (the jump in the normal derivative is penalized)
- Wheeler(78) (IP collocation-FEM), Arnold(79), Douglas et al.(79)
- Oden, Babuška, and Baumann(1998); Rivière and Wheeler(00)
- Houston, Schwab, and S*ü*li(00); Epshteyn, Rivière(06)
- WG: Wang JP, Ye X, Mu L, Zhang SY, Zhang R, Zhai QL, Zhang ZM, Wang CM, Xie XP, Gao FZ, Cheng JR, Wang XS etc.
- NPB: Cheng YD, Shu CW(09, 11, 17); Peng, Huang YQ, Liu HL(iterative DG for PB, 14, 18); Xu, Zhao(DG for NPB, 15)
- Kwon, Kwak(Discontinuous bubble immersed FEM for PB 19; PBNB 21)

References

- Maccamy, Suri, A time-dependent interface problem for two-dimensional eddy currents, Quart Appl Math (87)
- Jianguo Huang, Jun Zou, Some new a priori estimates for second-order elliptic and parabolic interface problems, JDE (02)
- Khan, Upadhyay, Gerritsma, Spectral element methods for parabolic interface problems, CMAME (18)
- Derrick Johns, Xu Zhang, High order immersed FEM for parabolic interface problems with time variable in 1D, ITM conference (19)
- Ruchi Guo, backward Euler+IFE, Parabolic moving interface problems with dynamical immersed spaces on unfitted meshes, SINUM (20).
- Ajerid, Babuska, Guo, Lin, (higher degree IFE for elliptic interface problem), An enriched immersed FEM for interface problems with nonhomogeneous jumps conditions, CMAME (23)
- ...

WG finite element method for elliptic equations

PDE weak form: find $u \in H_0^1(\Omega)$ satisfying

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

The WG method: element $(P_k(T), P_j(e), [P_s(T)]^d)$ find $u_h \in V_h$ such that

$$(a\nabla_w u_h, \nabla_w v_h) + s(u_h, v_h) = (f, v_h), \quad ,\forall v_h \in V_h,$$

$$s(u_h, v) = \sum_T h^j \langle u_0 - u_b, v_0 - v_b\rangle_{\partial T}, \quad j = -1, 0, 1, \infty, \leq -1(relaxed)$$

$$V_h = \{v = v_0, v_b : v_0|_T \in P_k(T), v_b|_e \in P_j(e), e \subset \partial T, \forall T \in \mathcal{T}\}$$

For $v = \{v_0, v_b\} \in V_h$, $\nabla_w v|_T \in [P_s(T)]^d$ satisfies

$$(\nabla_w v, \tau) = -(v_0, \nabla \cdot \tau)_T + \langle v_b, \tau \cdot \mathbf{n}\rangle_{\partial T}, \quad ,\forall \tau \in [P_s(T)]^d,$$

[1] J. Wang, X. Ye, S. Zhang, Numerical investigation on weak Galerkin finite elements. Int. J. Numer. Anal. Model. 17 (2020), no. 4, 517-531.

Open problem: superconvergence/optimal convergence on element $(P_k(T), P_k(e), RT_k(T)]^d)$ on triangular mesh, $j = -1, 0, 1$, has not been proved. (see [1] Table 4.4)

WG method and Stabilizer-Free WG (SFWG)

WG finite element: $(P_k(T), P_{k-1}(e), [P_{k-1}]^d)$
The WG method: find $u_h \in V_h$ such that for any $v_h \in V_h$

$$(a\nabla_w u_h, \nabla_w v_h) + s(u_h, v_h) = (f, v_h),$$

The SFWG method: find $u_h \in V_h$ such that for any $v_h \in V_h$

$$(a\nabla_w u_h, \nabla_w v_h) = (f, v_h),$$

SFWG finite element: $(P_k(T), P_k(e), [P_{k+n-1}]^d)$, n : #sides

[2] X.Ye, S. Zhang, A stabilizer-free weak Galerkin finite element method on polytopal meshes, J. Comput. Appl. Math., 372(2020), 112699.

Open problem: Is $k+n-1$ optimal? Sufficient but not necessary condition.

Modified Weak Galerkin (MWG)

Idea: replace v_b by $\{v\}$, only involving the interior function v.
Set $V_h = \{v \in L^2(\Omega) : v|_T \in P_k(T), \forall T \in \mathcal{T}_h\}$.
The MWG method: find $u_h \in V_h$ such that for any $v_h \in V_h$

$$(a\nabla_w u_h, \nabla_w v_h) + s(u_h, v_h) = (f, v_h),$$

For $v \in V_h$, $\nabla_w v|_T \in [P_{k-1}(T)]^d)$ satisfies

$$(\nabla_w v, \tau) = -(v, \nabla \cdot \tau)_T + \langle \{v\}, \tau \cdot \mathbf{n} \rangle_{\partial T}, \quad , \forall \tau \in [P_{k-1}(T)]^d,$$

MWG element: $\{P_k(T), [P_{k-1}]^2\}$

[3] X. Wang, N. Malluwawadu, F. Gao and T. McMillan, A modified weak Galerkin finite element method, J. Comput. Appl. Math., 217 (2014), 319-327.

Modified Weak Galerkin (MWG)

The MWG method

$$(a\nabla_w u_h, \nabla_w v_h) + s(u_h, v_h) = (f, v_h),$$

$$(\nabla_w v, \tau) = -(v, \nabla\cdot\tau)_T + \langle \{v\}, \tau\cdot\mathbf{n}\rangle_{\partial T}, \quad ,\forall \tau \in [P_{k-1}(T)]^d,$$

[3] X. Wang, N. Malluwawadu, F. Gao and T. McMillan, A modified weak Galerkin finite element method, J. Comput. Appl. Math., 217 (2014), 319-327.

Note that there are many different ways to replace v_b besides $v_b = \{v\}$.

Recall the LDG method: find $\mathbf{q}_h \in \mathbf{V}_h$, $u_h \in W_h$ such that

$$\begin{aligned}(a^{-1}\mathbf{q}_h, \mathbf{v}) + (\nabla\cdot\mathbf{v}, u_h)_{\mathcal{T}_h} - \langle \hat{u}_h, \mathbf{v}\cdot\mathbf{n}\rangle_{\partial\mathcal{T}_h} &= 0, \quad \forall \mathbf{v} \in \mathbf{V}_h \\ (\mathbf{q}_h, \nabla w)_{\mathcal{T}_h} - \langle \hat{\mathbf{q}}_h\cdot\mathbf{n}, w\rangle_{\partial\mathcal{T}_h} &= (f, w), \quad \forall w \in W_h\end{aligned}$$

where $\hat{u}_h = \{u_h\} - \beta\cdot[u_h]$ and $\hat{\mathbf{q}}_h = \{\mathbf{q}_h\} + \beta[\mathbf{q}_h] - \alpha[u_h]$.

HDG finite element method

Recall the HDG method: find $(\mathbf{q}_h, u_h, \hat{u}_h) \in \mathbf{V}_h \times W_h \times M_h$ such that

$$\begin{aligned}
(a^{-1}\mathbf{q}_h, \mathbf{v}) - (u_h, \nabla\cdot\mathbf{v})_{\mathcal{T}_h} + \langle \hat{u}_h, \mathbf{v}\cdot\mathbf{n}\rangle_{\partial\mathcal{T}_h} &= 0, \quad \forall \mathbf{v} \in \mathbf{V}_h \\
-(\mathbf{q}_h, \nabla w)_{\mathcal{T}_h} + \langle \hat{\mathbf{q}}_h\cdot\mathbf{n}, w\rangle_{\partial\mathcal{T}_h} &= (f, w), \quad \forall w \in W_h \\
\langle \hat{\mathbf{q}}_h\cdot\mathbf{n}, \mu\rangle_{\partial\mathcal{T}_h n \partial\Omega} &= 0, \quad \forall \mu \in M_h, \\
\langle \hat{u}_h, \mu\rangle_{\partial\Omega} &= 0, \quad \forall \mu \in M_h, \\
\hat{\mathbf{q}}_h\cdot\mathbf{n} &= \mathbf{q}_h\cdot\mathbf{n} + \tau(u_h - \hat{u}_h).
\end{aligned}$$

To solve a function $\hat{u}_h$ in HDG is analogous to find an alternative of $\{v\}$ in the MWG method.

Approximation spaces $(P_k, [P_{k-1}(e)]^2, [P_{k-1}(K)]^d)$

$$
\begin{aligned}
V_h :=& \{(v_0, v_b) : v_0 |_K \in P_k(K), K \in \mathcal{T}_h; v_b |_e \in [P_{k-1}(e)]^2, e \in \mathcal{E}_I; \\
& \quad v_b |_e \in P_{k-1}(e), e \in \partial\Omega \cup \Gamma, k \geq 1\}, \\
V_h^0 :=& \{v \in V_h, v_b = 0 \text{ on } \partial\Omega \backslash \Gamma\}.
\end{aligned}
$$

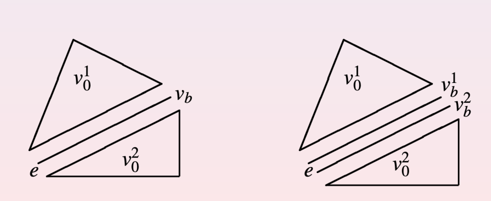


Figure: L: single-valued; R: double-valued

The discrete weak gradient space: $RT_k(K)$, $k \geq 0$,
The weak Galerkin finite element space

$$V_h = \{(v_0,\ v_b) : v_{0|K} \in \mathbb{P}_k(K),\ K \in \mathcal{T}_h;$$
$$v_{b|e} \in \mathbb{P}_k(e) \times \mathbb{P}_k(e),\ \forall e \in \mathcal{E}_h^I;\ v_{b|e} \in \mathbb{P}_k(e),\ \forall e \in \mathcal{E}_h^B\},$$

Element $(\mathbb{P}_k, [\mathbb{P}_k]^2, RT_k)$:

$$a_{opwg}(w,v) := (A\nabla_w w, \nabla_w v) + \sum_{e\in\mathcal{E}_{\mathcal{I}}} |e|^{-\beta_0} \langle [\![w_b]\!], [\![v_b]\!]\rangle_e.$$

A New Over-Penalized WG method

part I. Liu, Song, Zhao, Discrete Contin. Dyn. Syst. Ser. B, 26 (2021), 2411-2428

part II. Song, Qi, Liu, Gu, Discrete Contin. Dyn. Syst. Ser. B, 26 (2021), 2581-2598

$$\begin{aligned} V_h = \{(v_0,\ v_b) : v_0|_K \in \mathbb{P}_k(K),\ K \in \mathcal{T}_h, \\ v_b|_e \in \mathbb{P}_j(e) \times \mathbb{P}_j(e), e \in \mathcal{E}_{\mathcal{I}};\ v_b|_e \in \mathbb{P}_j(e), e \in \partial\Omega\}, \quad j = k,\ k-1, \\ V_h^0 = \{(v_0,\ v_b) : v \in V_h,\ v_b = 0 \text{ on } \partial\Omega\}, \end{aligned}$$

Element $(\mathbb{P}_k(K), [\mathbb{P}_j(e)]^2, [\mathbb{P}_{k-1}(K)]^2)$: To find $u_h = (u_0, u_b) \in V_h$ s.t.

$$a_{opwg}(u_h, v) = (f, v_0), \quad \forall\, v = (v_0, v_b) \in V_h, \tag{1}$$

where

$$a_{opwg}(w, v) := (A\nabla_w w, \nabla_w v) + s(w, v) + \sum_{e \in \mathcal{E}_{\mathcal{I}}} |e|^{-\beta_0} \langle [\![w_b]\!], [\![v_b]\!] \rangle_e,$$

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

- The parabolic interface problem

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ be a convex polygon or polyhedral domain, $\Omega_1 \subset \Omega$ be an open domain with Lipschitz continuous boundary $\Gamma = \partial\Omega_1 \subset \Omega$, and $\Omega_2 = \Omega \setminus \overline{\Omega}_1$.

$$\begin{cases} u_t - \nabla \cdot (A\nabla u) = f(x,t) & \text{in } \Omega \times (0, T], \\ u(x,0) = \varphi(x) & \text{in } \Omega, \\ u = g(x,t) & \text{on } \partial\Omega \setminus \Gamma \times (0, T], \\ [\![u]\!]_\Gamma = \psi(x,t) & \text{on } \Gamma \times (0, T], \\ [\![A\nabla u \cdot \mathbf{n}]\!]_\Gamma = \phi(x,t) & \text{on } \Gamma \times (0, T], \end{cases} \tag{2}$$

$A := A(x, t)$ s.p.d. matrix-valued function or a piecewise positive function.
$[\![u]\!]_\Gamma := u|_{\partial\Omega_1 \cap \Gamma} - u|_{\partial\Omega_2 \cap \Gamma}$
$[\![A\nabla u \cdot \mathbf{n}]\!]_\Gamma := A\nabla u|_{\Omega_1} \cdot \mathbf{n}_1 + A\nabla u|_{\Omega_2} \cdot \mathbf{n}_2$.

Meshes in Example 1

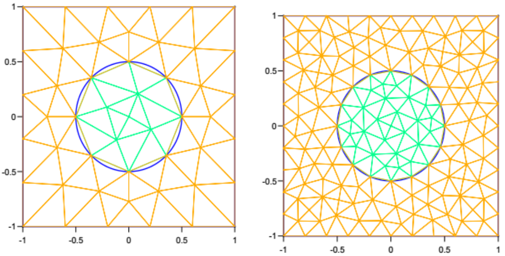


Figure: Meshes used in Example 1: (left) h=2/5, (right) h=1/5

Convergence rates (h) in Example 1

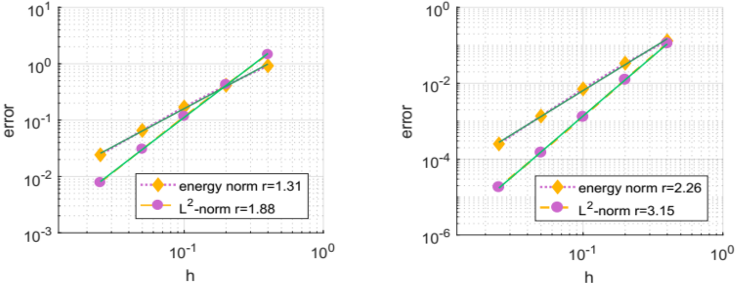


Figure: Example 1. Convergence w.r.t h: (Left) $k = 1$, (Right) $k = 2$

Convergence rates (τ) in Example 1

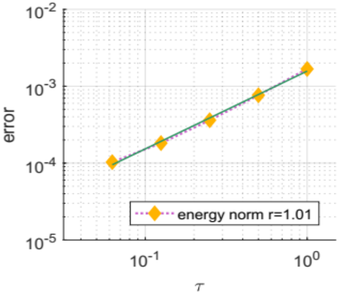


Figure: Example 1. Convergence w.r.t τ: (Left) $k = 1$, (Right) $k = 2$

Meshes in Example 2

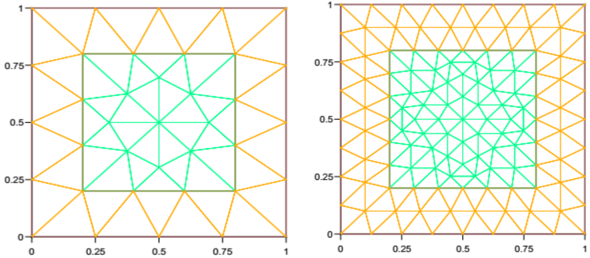


Figure: Meshes used in Example 2: (left) $h=2/5$, (right) $h=1/5$

Convergence rates (h) in Example 2

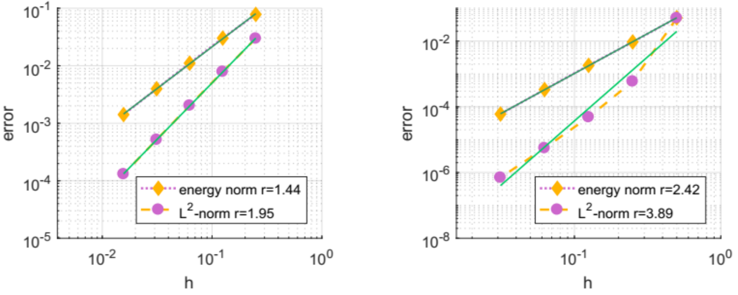
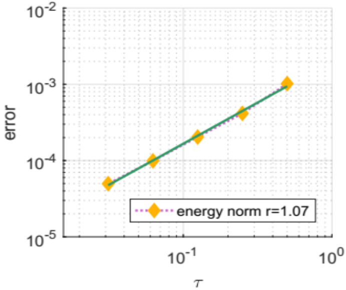


Figure: Example 2. Convergence w.r.t h: (Left) $k = 1$, (Right) $k = 2$

Convergence rates (τ) in Example 2



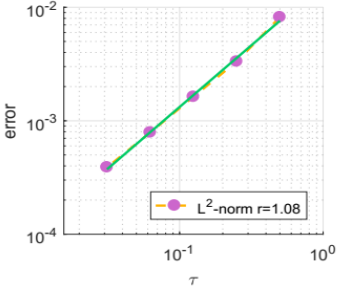


Figure: Example 2. Convergence w.r.t τ: (Left) $k = 1$, (Right) $k = 2$

- Stationary convection diffusion reaction problem

$$
\begin{aligned}
&-\nabla\cdot(A\nabla u)+\mathbf{b}\cdot\nabla u+cu=f, \quad \text{in } \Omega,\\
&u=0, \quad \text{on } \partial\Omega.
\end{aligned}
$$

$A:=(a_{ij}(\mathbf{x}))\in[L^\infty(\Omega)]^{d\times d}$ s.p.d matrix-valued function;
$\mathbf{b}=(b_i(\mathbf{x}))_{d\times 1}\in[W^{1,\infty}(\Omega)]^d$ and $c=c(\mathbf{x})\in L^\infty(\Omega)$;

$$
c_0(x):=c(\mathbf{x})-\frac{1}{2}\nabla\cdot\mathbf{b}(\mathbf{x})\geq 0, \qquad \forall\,\mathbf{x}\in\Omega.
$$

Discrete approximation space: $(\mathbb{P}_k(T), \mathbb{P}_k^2(e), \mathbb{P}_{k-1}(T)^d)$

Def. $(\mathbf{b}\cdot\nabla_w)v_h \in \mathbb{P}_k(T), \forall\, \phi_h \in \mathbb{P}_k(T)$,

$$((\mathbf{b}\cdot\nabla_w)v_h, \phi_h)_T = -(\mathbf{b}\cdot\nabla\phi_h, v_0)_T - ((\nabla\cdot\mathbf{b})\phi_h, v_0)_T + \langle \phi_h v_b, \mathbf{b}\cdot\mathbf{n}\rangle_{\partial T}$$

$$(A\nabla_w v, \nabla_w w) + \frac{1}{2}((\mathbf{b}\cdot\nabla_w)v, w_0) - \frac{1}{2}((\mathbf{b}\cdot\nabla_w)w, v_0) + (c_0 v_0, w_0)$$
$$+ s(v,w) + J(v,w) = (f, v), \qquad \forall\, v \in V_h^0,$$

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

$$J(v,w) := \sum_{e\in\mathcal{E}_{\mathcal{I}}} |e|^{-\beta_0}\langle [\![v_b]\!], [\![w_b]\!]\rangle_e.$$

When $\beta_0 \geq 2k+1$, the error estimates in the energy and L^2 norms are optimal with the convergence rates k and $k+1$, respectively.

- Convection diffusion reaction problem with variable coefficients

$(\mathbb{P}_k(T),\ [\mathbb{P}_k(e)]^2,\ [\mathbb{P}_{k-1}(T)]^2), k = 1, 2;$
(1) L-shaped domain. Let $\Omega = (-1,1)^2 \setminus (0,1) \times (-1,0)$, and set $u(x,y) = \sin(\pi x)\sin(\pi y)$ and
$A = \mathrm{diag}([2,3]), \quad \mathbf{b} = [1,-1]^{\mathrm{T}}, \quad c = \sin(xy).$

Table: L-shaped domain.

	h	$\|\|\|e_h\|\|\|$	rates	$\|\|e_0\|\|$	rates
	1/8	6.1262e+00	-	1.0837e+00	-
$k=1$	1/16	3.1637e+00	0.9533	2.8710e-01	1.9163
$\beta_0 = 3$	1/32	1.6016e+00	0.9820	7.3398e-02	1.9677
	1/64	8.0463e-01	0.9931	1.8508e-02	1.9875
	1/128	4.0310e-01	0.9971	4.6435e-03	1.9948
	1/8	1.5931e+00	-	1.0745e-01	-
$k=2$	1/16	4.0802e-01	1.9163	1.2024e-02	3.1596
$\beta_0 = 5$	1/32	1.0273e-01	1.9677	1.4513e-03	3.0504
	1/64	2.5764e-02	1.9875	1.7971e-04	3.0136
	1/128	6.4507e-03	1.9948	2.2406e-05	3.0037

- Convection diffusion reaction problem with variable coefficients

$(\mathbb{P}_k(T),\ [\mathbb{P}_k(e)]^2,\ [\mathbb{P}_{k-1}(T)]^2), k = 1, 2;$

(2) Interior layer. R Lin, X Ye, S Zhang and P Zhu, WG for Singularly Perturbed Convection-Diffusion-Reaction Problems, SINUM, 2018.

Let $\Omega = (0,1)^2$, and set $u(x,y) = 0.5x(1-x)y(1-y)(1-\tanh(\frac{\eta-x}{\gamma}))$ and $A = \mathrm{Id}/10, \quad \mathbf{b} = [1,0]^{\mathrm{T}}, \quad c = 1.$

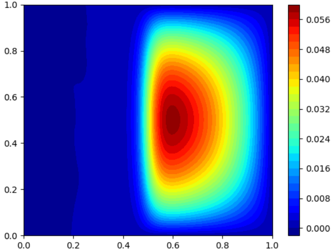


Figure: WG solution (*Left*) Vs. exact solution (*Right*).

Completed work and applications on OPWG

(1) elliptic, elliptic interface, parabolic, parabolic interface problems as well as spatiotemporal diffusion coeffcients of variation;
(2) stationery convection-diffusion equations with variable coefficients;
(3) and stationery Navier-Stokes equation;
(4) propose an Immersed and Over-Penalized Weak Galerkin (IOPWG) for elliptic interface problem.

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1. Introduction
2. Several variants of weak Galerkin methods ($p = 2$)
3. Over-Penalized Weak Galerkin (OPWG) method
4. Introduction to Relaxed Weak Galerkin (RWG) Method ($p \in (1, 2]$)

Problem:

Given $f \in L^p$, find $u \in W^{2,p} \cap H_0^1(\Omega)$, $p \in (1,2)$ such that

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

[Wihler & Rivière, J Sci Comput,2011], convergence rates of SIPG and NIPG schemes deteriorate when p is close to 1, even for the WG method with a stabilizer

$$S(u_h, v_h) = \sum_{e\in\mathcal{E}_h} h^{-1}\langle u_0 - u_b, v_0 - v_b\rangle_e.$$

Motivation: How to solve the low regularity problem well?

Elliptic interface problems

To find u satisfying

$$
\begin{aligned}
&-\nabla\cdot A_1\nabla u = f_1, && \text{in } \Omega_1, && (3)\\
&-\nabla\cdot A_2\nabla v = f_2, && \text{in } \Omega_2, && (4)\\
&u = g_1, && \text{on } \partial\Omega_1\setminus\Gamma, && (5)\\
&v = g_2, && \text{on } \partial\Omega_2\setminus\Gamma, && (6)\\
&u\big|_{\Omega_1} - v\big|_{\Omega_2} = \phi, && \text{on } \Gamma, && (7)\\
&A_1\nabla u|_{\Omega_1}\cdot\mathbf{n_1} + A_2\nabla v|_{\Omega_2}\cdot\mathbf{n_2} = \psi, && \text{on } \Gamma, && (8)
\end{aligned}
$$

where subdomains Ω_1, Ω_2 : open bounded polygonal domain in $\mathbb{R}^2$; coefficients A_i $(i = 1, 2)$ are positive in Ω_i; $\Gamma = \overline{\Omega}_1 \cap \overline{\Omega}_2$; $\mathbf{n_i}$ are unit normals exterior to Ω_i; $g_i \in H^{\frac{1}{2}}(\Omega)$; $\phi \in L^2(\Gamma)$; $\psi \in L^2(\Gamma)$; and $f_i \in L^p(\Omega_i)$ $(i = 1, 2)$ are given scalar-valued functions for some p in $(1, \infty]$.

Discrete weak gradient

Define $\nabla_w v \in [\mathbb{P}_{k-1}(T)]^2$ $(k \geq 1)$ for any function $v \in V_h$ satisfying

$$(\nabla_w v, q)_T = -(v_0, \nabla \cdot q)_T + \langle v_b, q \cdot \boldsymbol{n} \rangle_{\partial T}, \quad \forall\, q \in [\mathbb{P}_{k-1}(T)]^2.$$

Weak Galerkin element: $(\mathbb{P}_k(T), \mathbb{P}_k(e), [\mathbb{P}_{k-1}(T)]^2)$.

A natural finite element formulation for discontinuous elements should have the forms

$$a_i(u_h, v_h) := (A_i \nabla_w u_h, \nabla_w v_h) + S_i(u_h, v_h) = (f_i, v_h), \tag{9}$$

where the stabilizers

$$S_i(u_h, v_h) = \sum_{e \in \mathcal{E}_h^i} \frac{1}{h^\beta} \langle u_0 - u_b, v_0 - v_b \rangle_e, \; i = 1, 2,$$

where β is to be defined. Question: Does it depend on p?

The relaxed weak Galerkin (RWG) method

A numerical approximation with Lagrange multipliers for (3)-(8) can be obtained by seeking $u_h = (u_0, u_b) \in U_h$ satisfying $u_b = Q_b g_1$ on $\partial\Omega_1 \setminus \Gamma$, $v_h = (v_0, v_b) \in W_h$ satisfying $v_b = Q_b g_2$ on $\partial\Omega_2 \setminus \Gamma$ and $\lambda_h \in \Lambda_h$ such that

$$a_1(u_h, \omega) - \langle \lambda_h, \omega_b \rangle_\Gamma = (f_1, \omega_0), \quad \forall\, \omega \in U_h^0, \tag{10}$$

$$a_2(v_h, \rho) + \langle \lambda_h, \rho_b \rangle_\Gamma = (f_2, \rho_0) + \langle \psi, \rho_b \rangle_\Gamma, \quad \forall\, \rho \in W_h^0, \tag{11}$$

$$\langle u_b - v_b, \mu \rangle_\Gamma = \langle \phi, \mu \rangle_\Gamma, \quad \forall\, \mu \in \Lambda_h. \tag{12}$$

[7] Song, Qi, Liu, Gu, Applied Numerical Mathematics, 128(2018) 65-80.

Numerical settings

RWG: piecewise linear elements $(\mathbb{P}_1(T), \mathbb{P}_1(e), [\mathbb{P}_0(T)]^2)$

$$
\begin{aligned}
&L^2\text{-norm}: \ \|e_h\|^2 = \|e_0^1\|^2_{L^2(\mathcal{T}_h^1)} + \|e_0^2\|^2_{L^2(\mathcal{T}_h^2)},\\
&H^1\text{-norm}: \|\nabla_w e_h\|^2 = \|\nabla_w e_h^1\|^2_{L^2(\mathcal{T}_h^1)} + \|\nabla_w e_h^2\|^2_{L^2(\mathcal{T}_h^2)},\\
&L^\infty\text{-norm}: \ \|e_h\|_{L^\infty} = \max\left\{\|e_h^1\|_{L^\infty(\mathcal{T}_h^1)}, \|e_h^2\|_{L^\infty(\mathcal{T}_h^2)}\right\},\\
&\text{Energy norm: } |||\, e_h|||^2 = (A\nabla_w e_h, \nabla_w e_h)_{\mathcal{T}_h^1\cup\mathcal{T}_h^2} + \sum_{e\in\mathcal{E}_h} \frac{1}{h^\beta}\|Q_0 e_0 - e_b\|_e^2.
\end{aligned}
$$

Numerical results for low regularity elliptic problems

RWG: element $(\mathbb{P}_1(T), \mathbb{P}_1(e), [\mathbb{P}_0(T)]^2)$
Example 0. [Wihler & Rivière, J Sci Comput, 2011],

$$\Omega = (0,1)^2, \quad A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and the exact solution

$$u(x,y) = x(x-1)y(y-1)r^{-2+\alpha},$$

$\alpha \in (0,1]$ is a constant, and $r = \sqrt{x^2+y^2}$. Here

$$u \in H_0^1(\Omega) \cap W^{2,p}(\Omega), \quad p \in (1, \frac{2}{2-\alpha}) \subseteq (1,2).$$

Song, Liu, Zhao, J. Sci. Comput. 71 (2017), no. 1, 195-218.

WG solutions with low regularity

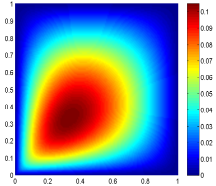


Figure: $\alpha = 1$

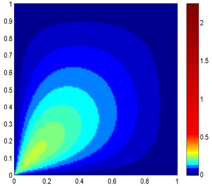


Figure: $\alpha = 2^{-2}$

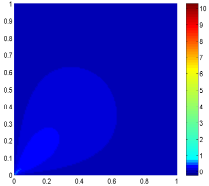


Figure: $\alpha = 2^{-5}$

Comparisons

Table: Convergence rates of $|||e_h|||$ with different methods.

α	SIPG	NIPG	FEM	$\underset{\beta=1}{\underline{\text{WG}}}$	$\underset{\beta=2}{\underline{\text{WG}}}$	$\underset{\beta=3}{\underline{\text{WG}}}$
1	0.905	0.918	0.924	0.8909	1.1872	1.4420
2^{-1}	0.491	0.494	0.500	0.4889	0.8998	0.9642
2^{-2}	0.245	0.247	0.249	0.2424	0.7039	0.8104
2^{-3}	0.121	0.122	0.124	0.1175	0.5917	0.7439
2^{-4}	0.0587	0.0602	0.0618	0.0550	0.5326	0.7119

A strategy to reduce the ill-conditioned effect

ILU preconditioning+restarted GMRES

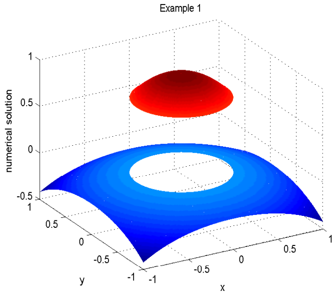
Example 1. Elliptic interface problem

In the domain $\Omega = (-1,1)^2$ with a circular interface $r^2 := x^2 + y^2 = 0.25$; $A_1 = b$ and $A_2 = 2$, respectively, on each subdomain satisfying $r > 0.5$ and $r \leq 0.5$. The analytical solution is

$$\begin{cases} u(x,y) = -\frac{1}{b}\left[\frac{1}{4}\left(1 - \frac{1}{8b} - \frac{1}{b}\right) + \left(\frac{r^4}{2} + r^2\right)\right], & r > 0.5, \\ v(x,y) = -(x^2 + y^2 - 1), & r \leq 0.5, \end{cases}$$

where $b = 10$. The corresponding force term can be derived, i.e., $f = 8r^2 + 4$ as $r > 0.5$, and $f = 8$ as $r \leq 0.5$. On the interface boundary, the corresponding functions $\psi = 4r^2(r^2 - 1)$ and ϕ along the interface are derived.

Convergence rates for Example 1



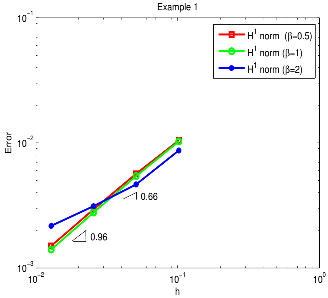


Figure: Numerical solu. (left) and $\|\nabla_w e_h\|_{L^2}$ (right) for $\beta = 0.5,\ 1,\ 2$.

Convergence rates and errors

Table: Example 1 with $\beta = 1$, 2.

$\max\{h\}$	$\beta=1$			$\beta=2$		
	$\|\|\|e_h\|\|\|$	$\|\nabla_w e_h\|$	$\|e_h\|$	$\|\|\|e_h\|\|\|$	$\|\nabla_w e_h\|$	$\|e_h\|$
0.1018	9.4660e-1	1.0269e-2	2.1495e-2	3.0703e-1	8.6956e-3	2.6167e-3
0.0509	4.7285e-1	5.4263e-3	5.3688e-3	9.5458e-2	4.6587e-3	2.8571e-4
0.0255	2.3634e-1	2.7763e-3	1.3400e-3	3.0803e-2	3.1209e-3	3.1964e-5
0.0128	1.1815e-1	1.4031e-3	3.3523e-4	1.7835e-2	2.1707e-3	6.6414e-6
Rate	1.0038	0.9612	2.0073	1.3990	0.6605	2.9115

Example 2. Elliptic interface problem

In the domain $\Omega = (0,1)^2$ with a circular interface $r^2 = (x-0.5)^2 + (y-0.5)^2 = 0.25^2$, the coefficient A is defined to be $A_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and $A_2 = 2$, respectively on each subdomain, for $r > 0.25$ and $r \leq 0.25$. The analytical solution is

$$\begin{cases} u(x,y) = x(x-1)y(y-1)r^{-2+\alpha}, & r > 0.25, \\ v(x,y) = 1-(2x-1)^2-(2y-1)^2, & r \leq 0.25, \end{cases}$$

where $\alpha \in (0,1]$ is a constant, and $r = \sqrt{x^2+y^2}$ denotes the distance to the origin. Here

$$u \in H_0^1(\Omega) \cap W^{2,p}(\Omega) \quad \text{for} \quad p \in (1, \frac{2}{2-\alpha}) \subseteq (1,2).$$

Convergence rates and errors

Table: Convergence rates and errors for example 2 with $\beta = 1$, 1.5, and $\alpha = 2^{-4}$ taken.

	$\beta = 1$		$\beta = 1.5$	
$\max\{h\}$	$\|\|\|e_h\|\|\|$	$\|\|e_h\|\|$	$\|\|\|e_h\|\|\|$	$\|\|e_h\|\|$
0.0509	6.0075e+0	6.2693e-2	2.7505e+0	1.4089e-2
0.0255	5.7696e+0	3.0076e-2	2.0746e+0	4.3410e-3
0.0128	5.5343e+0	1.4414e-2	1.5214e+0	1.3648e-3
0.0064	5.3046e+0	6.9078e-3	1.0880e+0	4.7494e-4
Rate	0.0601	1.0640	0.4476	1.6392

Convergence rates for Example 2

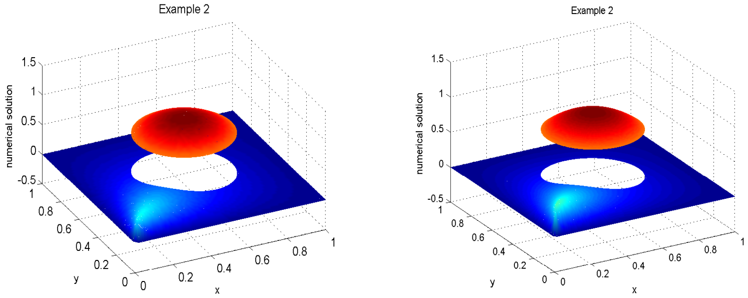


Figure: Numerical solu. $\alpha = 2^{-4}$ (left) and numerical solu. with $\alpha = 2^{-6}$ (right).

Convergence rates for Example 2

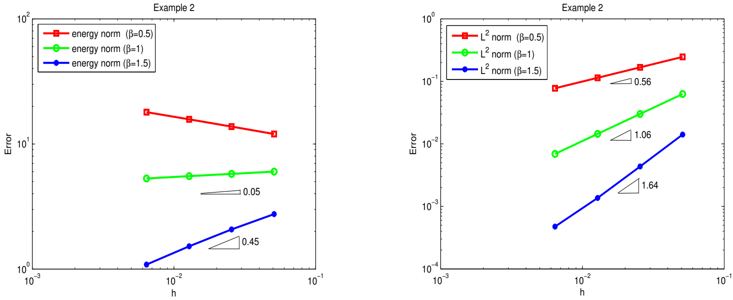


Figure: In the case $\alpha = 2^{-4}$, convergence rates of $|||e_h|||$ (left) and $\|e_h\|$ (right) with $\beta = 0.5,\ 1,\ 1.5$ taken.

Example 3. Elliptic interface problem

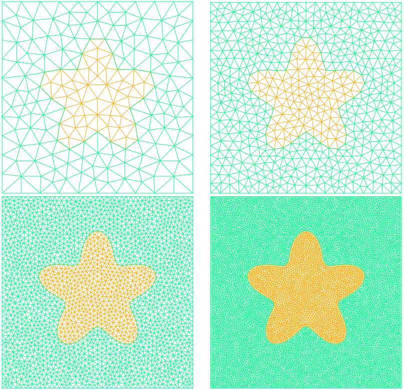
We consider a classical elliptic interface problem in the domain $\Omega = (-1, 1)^2$ with both concave and convex curve segments appeared in (see [Zhou, Wei 2006]). The interface is parametrized with the polar angle θ by

$$r = \frac{1}{2} + \frac{1}{7}\sin(5\theta).$$

The coefficients $A_1 = 10$ and $A_2 = 1$ are chosen for the subdomains outside Γ and inside Γ, respectively. The analytic solution is given as

$$\begin{cases} u(x,y) = \frac{1}{10}(x^2+y^2)^2 - \frac{1}{100}\ln(\sqrt{2(x^2+y^2)}), & \text{in } \Omega_1, \\ v(x,y) = \exp(x^2+y^2), & \text{in } \Omega_2, \end{cases}$$

Refined meshes with a curved interface



Convergence rates for Example 3

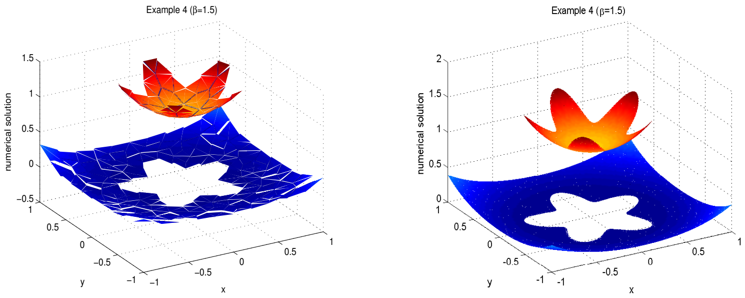


Figure: Numerical solutions on mesh level 1 (left) and on mesh level 4 (right).

Convergence rates for Example 3

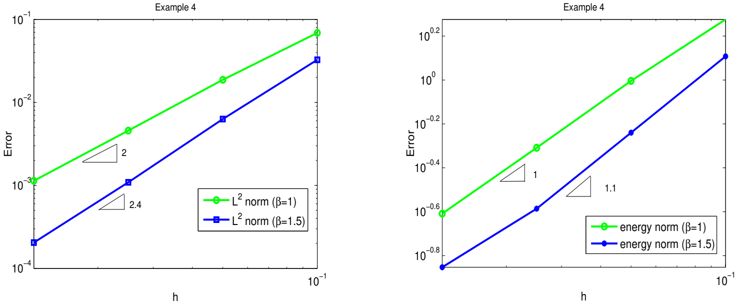


Figure: Convergence rates of $\|e_h\|$ (left) and $|||e_h|||$ (right) for $\beta = 1$, 1.5 in Example 3.

Example 4

Let $\Omega = [0,1] \times [0,1]$, the coefficient

$$A(\boldsymbol{x}/\epsilon) = \frac{1}{4 + P(\sin(2\pi x/\epsilon) + \sin(2\pi y/\epsilon))},$$

where P is a controlling parameter of the magnitude for the oscillation. We apply $P = 1.8$. The exact solution is given

$$u = \frac{\sqrt{4 - P^2}}{2}(x^2 + y^2).$$

Example 4 [Mu, Wang, Ye, A weak Galerkin generalized multiscale FEM, JCAM, (305)2016, 68-81]

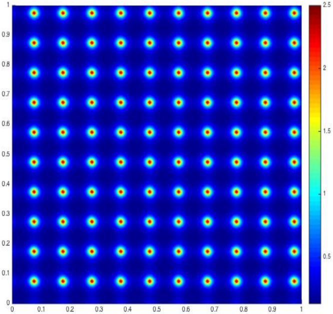


Figure: Multiscale coefficients, $\epsilon = 0.1$.

Convergence rates for Example 4 ($\epsilon = 0.1$)

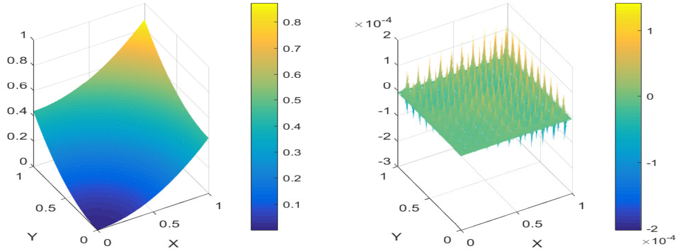


Figure: Numerical solution (left) and error (right).

Convergence rates for Example 4 ($\epsilon = 0.1$)

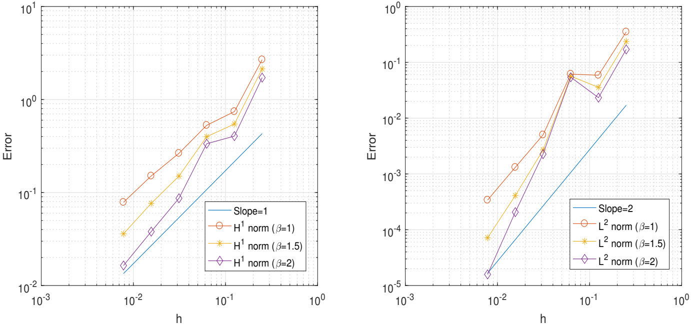


Figure: Convergence rates of $\|e_h\|$ (left) and $|||e_h|||$ (right).

Conclusions

1. Several variants of WG finite element methods have been summerized.
2. In the case $p = 2$, the OPWG methods are introduced.
3. The relaxed weak Galerkin method is suitable for solving low regularity elliptic problem and elliptic interface problem ($p \in (1, 2]$).