isoGeometric Residual Minimization Method (iGRM)

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Marcin Łoś, Ph.D. Research interests: fast solvers for time-dependent simulations (advection-diffusions, non-linear flow, Stokes problem, wave propagation), C++

Maciej Woźniak, Ph.D. Research interests: parallel computing, alternating direction solvers, models of concurrency, computational cost, MPI+openMP, Fortran

Konrad Jopek, M.Sc. Research interests: Linux cluster administration, code optimization, multi-frontal direct solvers, C++, Fortran

Grzegorz Gurgul, M.Sc. Research interests: cloud computing, object-oriented solvers, simulations (flood simulations, Cahn-Hilliard simulations), web-interfaces, JAVA

Krzysztof Podsiadło, M.Sc. Research interests: mesh generation algorithms, graph grammars, pollution simulations, C++

Software

Program Title: **IGA-ADS**
(Isogeometric Analysis Alternating Directions Solver)
Code: `git clone https://github.com/marcinlos/iga-ads`

License: MIT license (MIT)   Programming language: C++
Nature of problem: Solving non-stationary problems in 1D, 2D and 3D with alternating direction solver and isogeometric analysis
Open source, parallel, flexible (2D/3D, multi-physics, stabilization: residual minimization, SUPG, DG, different time schemes)

[1] Marcin Łoś, Maciej Woźniak, Maciej Paszyński, Andrew Lenharth, Keshav Pingali *IGA-ADS : Isogeometric Analysis FEM using ADS solver*, **Computer & Physics Communications** 217 (2017) 99-116

[2] Marcin Łoś, Adriank Kłusek, M. Amber Hassaan, Keshav Pingali, Witold Dzwinel, Maciej Paszyński, *Parallel fast isogeometric L2 projection solver with GALOIS system for 3D tumor growth simulations*, **Computer Methods in Applied Mechanics and Engineering**, 343, (2019) 1-22

Outline

- Motivation
- isoGeometric Residual Minimization method (iGRM) for time-dependent problems
  - Different time integration schemes
  - Residual minimization method
  - Factorization of residual minimization problem matrix
  - Numerical results: manufactured solution, pollution from a chimney
- isoGeometric Residual Minimization method (iGRM) for stationary problems
  - Iterative solver
  - Numerical results: Manufactured solution problem, Eriksson-Johnson model problem
- Conclusions

Motivation

isogeometric Residual Minimization Method for time-dependent problems

isoGeometric Residual Minimization Method (iGRM)

- Second order time integration scheme
  (unconditional stability in time)
- Residual minimization for each time step
  (stability in space)
- Discretization with B-spline basis functions
  (higher continuity smooth solutions)
- Kronecker product structure of the matrix
  (linear cost $\mathcal{O}(N)$ of direct solver)

isogeometric Residual Minimization Method for stationary problems

isoGeometric Residual Minimization Method (iGRM)

- Residual minimization
  (stability in space)
- Discretization with B-spline basis functions
  (higher continuity smooth solutions)
- Kronecker product structure of the inner product matrix
  (linear cost $\mathcal{O}(N)$ preconditioner for iterative solver)
- Symmetric positive definite system
  (convergence of the conjugated gradient method)

Time-Dependent problems

Marcin Los, Judit Munoz-Matute, Ignacio Muga, Maciej Paszynski, Isogeometric Residual Minimization Method (iGRM) with Direction Splitting for Non-Stationary Advection-Diffusion Problems, submitted to *Computers and Mathematics with Applications* (2019) **IF: 1.861**

M. Los, J. Munoz-Matute, Keshav Pingali, Ignacio Muga, Maciej Paszynski, Parallel Shared-Memory Isogeometric Residual Minimization (iGRM) Simulations of 3D Advection-Diffusion Problems, submitted to *Engineering with Computers* (2019) **IF: 1.951**

Judit Munoz-Matute, Ms.C. The University of the Basque Country, Bilbao, Spain

Ignacio Muga, Professor of Mathematics, The Pontifical Catholic University of Valparaiso, Chile

Keshav Pingali, Professor of Computer Science, The University of Texas in Austin, USA

Mass and stiffness matrices over 2D domain $\Omega = \Omega_x \times \Omega_y$

$$\mathcal{M} = (B_{ij}, B_{kl})_{L^2} = \int_\Omega B_{ij} B_{kl} \,\mathrm{d}\Omega =$$

$$\int_\Omega B_i^x(x) B_j^y(y) B_k^x(x) B_l^y(y) \,\mathrm{d}\Omega = \int_\Omega (B_i B_k)(x)\,(B_j B_l)(y) \,\mathrm{d}\Omega$$

$$= \left(\int_{\Omega_x} B_i B_k \,\mathrm{d}x\right) \left(\int_{\Omega_y} B_j B_l \,\mathrm{d}y\right) = \mathcal{M}^x \otimes \mathcal{M}^y$$

$$\mathcal{S} = (\nabla B_{ij}, \nabla B_{kl})_{L^2} = \int_\Omega \nabla B_{ij} \cdot \nabla B_{kl} \,\mathrm{d}\Omega =$$

$$\int_\Omega \frac{\partial(B_i^x(x) B_j^y(y))}{\partial x} \frac{\partial(B_k^x(x) B_l^y(y))}{\partial x} + \frac{\partial(B_i^x(x) B_j^y(y))}{\partial y} \frac{\partial(B_k^x(x) B_l^y(y))}{\partial y} \,\mathrm{d}\Omega$$

$$= \int_\Omega \frac{\partial B_i^x(x)}{\partial x} B_j^y(y) \frac{\partial B_k^x(x)}{\partial x} B_l^y(y) + B_i^x(x) \frac{\partial B_j^y(y)}{\partial y} B_k^x(x) \frac{\partial B_l^y(y))}{\partial y} \,\mathrm{d}\Omega$$

$$= \int_{\Omega_x} \frac{\partial B_i}{\partial x} \frac{\partial B_k}{\partial x} \,\mathrm{d}x \int_{\Omega_y} B_j B_l \,\mathrm{d}y + \int_{\Omega_x} B_i B_k \,\mathrm{d}x \int_{\Omega_y} \frac{\partial B_j}{\partial y} \frac{\partial B_l}{\partial y} \,\mathrm{d}y$$

$$= \mathcal{S}^x \otimes \mathcal{M}^y + \mathcal{M}^x \otimes \mathcal{S}^y$$

Non-stationary advection-diffusion model

Let $\Omega = \Omega_x \times \Omega_y \subset \mathbb{R}^2$ a bounded domain and $I = (0, T] \subset \mathbb{R}$,

$$\begin{cases} \partial u/\partial t - \nabla \cdot (\alpha \nabla u) + \beta \cdot \nabla u = f & \text{in } \Omega \times I, \\ u = 0 & \text{on } \Gamma \times I, \\ u(0) = u_0 & \text{in } \Omega, \end{cases}$$

where Ω_x and Ω_y are intervals in $\mathbb{R}$. Here, $\Gamma = \partial\Omega$, $f : \Omega \times I \longrightarrow \mathbb{R}$ is a given source and $u_0 : \Omega \longrightarrow \mathbb{R}$ is a given initial condition.
We consider constant diffusivity α and a velocity field $\beta = [\beta_x \;\; \beta_y]$.

We split the advection-diffusion operator
$\mathcal{L}u = -\nabla \cdot (\alpha \nabla u) + \beta \cdot \nabla u$ as $\mathcal{L}u = \mathcal{L}_1 u + \mathcal{L}_2 u$ where

$$\mathcal{L}_1 u := -\alpha \frac{\partial u}{\partial x^2} + \beta_x \frac{\partial u}{\partial x}, \quad \mathcal{L}_2 u := -\alpha \frac{\partial u}{\partial y^2} + \beta_y \frac{\partial u}{\partial y}.$$

We perform an uniform partition of the time interval $\overline{I} = [0, T]$ as

$$0 = t_0 < t_1 < \ldots < t_{N-1} < t_N = T,$$

and denote $\tau := t_{n+1} - t_n, \; \forall n = 0, \ldots, N-1.$

Peaceman-Reachford scheme

$$
\begin{cases}
\dfrac{u^{n+1/2}-u^n}{\tau/2}+\mathcal{L}_1 u^{n+1/2}=f^{n+1/2}-\mathcal{L}_2 u^n,\\[2ex]
\dfrac{u^{n+1}-u^{n+1/2}}{\tau/2}+\mathcal{L}_2 u^{n+1}=f^{n+1/2}-\mathcal{L}_1 u^{n+1/2}.
\end{cases}
$$

$$
\begin{cases}
(u^{n+1/2},v)+\dfrac{\tau}{2}\left(\alpha\dfrac{\partial u^{n+1/2}}{\partial x},\dfrac{\partial v}{\partial x}\right)+\dfrac{\tau}{2}\left(\beta_x\dfrac{\partial u^{n+1/2}}{\partial x},v\right)=\\
(u^n,v)-\dfrac{\tau}{2}\left(\alpha\dfrac{\partial u^n}{\partial y},\dfrac{\partial v}{\partial y}\right)-\dfrac{\tau}{2}\left(\beta_y\dfrac{\partial u^n}{\partial y},v\right)+\dfrac{\tau}{2}(f^{n+1/2},v),\\[4ex]
(u^{n+1},v)+\dfrac{\tau}{2}\left(\alpha\dfrac{\partial u^{n+1}}{\partial y},\dfrac{\partial v}{\partial y}\right)+\dfrac{\tau}{2}\left(\beta_y\dfrac{\partial u^{n+1}}{\partial y},v\right)=\\
(u^{n+1/2},v)-\dfrac{\tau}{2}\left(\alpha\dfrac{\partial u^{n+1/2}}{\partial x},\dfrac{\partial v}{\partial x}\right)-\dfrac{\tau}{2}\left(\beta_x\dfrac{\partial u^{n+1/2}}{\partial x},v\right)+\dfrac{\tau}{2}(f^{n+1/2},v)
\end{cases}
$$

where $(\cdot,\cdot)$ denotes the inner product of $L^2(\Omega)$.

Peaceman-Reachford scheme (matrix form)

Finally, expressing problem in the Kronecker product matrix form we have

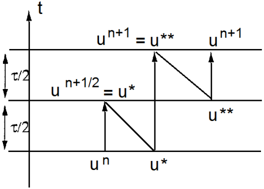
$$\begin{cases} \left[M^x + \frac{\tau}{2}(K^x + G^x)\right] \otimes M^y u^{n+1/2} = \\ \qquad M^x \otimes \left[M^y - \frac{\tau}{2}(K^y + G^y)\right] u^n + \frac{\tau}{2} F^{n+1/2}, \\ M^x \otimes \left[M^y + \frac{\tau}{2}(K^y + G^y)\right] u^{n+1} = \\ \qquad \left[M^x - \frac{\tau}{2}(K^x + G^x)\right] \otimes M^y u^{n+1/2} + \frac{\tau}{2} F^{n+1/2}, \end{cases}$$

where $M^{x,y}$, $K^{x,y}$ and $G^{x,y}$ are the 1D mass, stiffness and advection matrices, respectively.

In the Strang splitting scheme we divide problem $u_t + \mathcal{L}u = f$ into

$$\begin{cases} P_1 : u_t + \mathcal{L}_1 u = f, \\ P_2 : u_t + \mathcal{L}_2 u = 0, \end{cases}$$

the scheme integrates the solution from t_n to t_{n+1} into substeps:



$$\begin{cases} \text{Solve } P_1 : u_t + \mathcal{L}_1 u = f, \text{ in } (t_n, t_{n+1/2}), \\ \text{Solve } P_2 : u_t + \mathcal{L}_2 u = 0, \text{ in } (t_n, t_{n+1}), \\ \text{Solve } P_1 : u_t + \mathcal{L}_1 u = f, \text{ in } (t_{n+1/2}, t_{n+1}), \end{cases}$$

and we can employ different methods in each substep

Strang splitting scheme with Backward Euler method

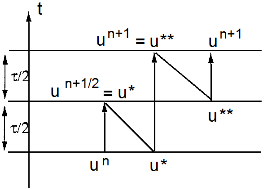
$$\begin{cases} \dfrac{u^{n+1/2} - u^n}{\tau/2} + \mathcal{L}_1 u^{n+1/2} = f^{n+1/2}, \\ \dfrac{u^{n+1} - u^n}{\tau} + \mathcal{L}_2 u^{n+1} = 0, \\ \dfrac{u^{n+1} - u^{n+1/2}}{\tau/2} + \mathcal{L}_1 u^{n+1} = f^{n+1}. \end{cases}$$

$$\begin{cases} (u^{n+1/2}, v) + \dfrac{\tau}{2}\left(\alpha \dfrac{\partial u^{n+1/2}}{\partial x}, \dfrac{\partial v}{\partial x}\right) + \dfrac{\tau}{2}\left(\beta_x \dfrac{\partial u^{n+1/2}}{\partial x}, v\right) \\ \quad = (u^n, v) + \dfrac{\tau}{2}(f^{n+1/2}, v), \\ (u^{n+1}, v) + \tau\left(\alpha \dfrac{\partial u^{n+1}}{\partial y}, \dfrac{\partial v}{\partial y}\right) + \tau\left(\beta_y \dfrac{\partial u^{n+1}}{\partial y}, v\right) = (u^n, v), \\ (u^{n+1}, v) + \dfrac{\tau}{2}\left(\alpha \dfrac{\partial u^{n+1}}{\partial x}, \dfrac{\partial v}{\partial x}\right) + \dfrac{\tau}{2}\left(\beta_x \dfrac{\partial u^{n+1}}{\partial x}, v\right) \\ \quad = (u^{n+1/2}, v) + \dfrac{\tau}{2}(f^{n+1}, v), \end{cases}$$

Strang splitting scheme with Backward Euler method

Expressing problem in the Kronecker product matrix form we have

$$\begin{cases} \left[M^x + \frac{\tau}{2}(K^x + G^x)\right] \otimes M^y u^* = M^x \otimes M^y u^n + \frac{\tau}{2} F^{n+1/2}, \\ M^x \otimes [M^y + \tau(K^y + G^y)]\, u^{**} = M^x \otimes M^y u^*, \\ \left[M^x + \frac{\tau}{2}(K^x + G^x)\right] \otimes M^y u^{n+1} = M^x \otimes M^y u^{**} + \frac{\tau}{2} F^{n+1}. \end{cases}$$



Strang splitting scheme with Crank-Nicolson method

If we select the Crank-Nicolson method for Strang scheme we obtain

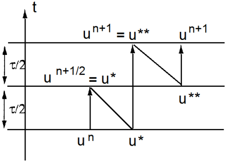
$$\begin{cases} \dfrac{u^{n+1/2} - u^n}{\tau/2} + \dfrac{1}{2}(\mathcal{L}_1 u^{n+1/2} + \mathcal{L}_1 u^n) = \dfrac{1}{2}(f^{n+1/2} + f^n), \\ \dfrac{u^{n+1} - u^n}{\tau} + \dfrac{1}{2}(\mathcal{L}_2 u^{n+1} + \mathcal{L}_2 u^n) = 0, \\ \dfrac{u^{n+1} - u^{n+1/2}}{\tau/2} + \dfrac{1}{2}(\mathcal{L}_1 u^{n+1} + \mathcal{L}_1 u^{n+1/2}) = \dfrac{1}{2}(f^{n+1} + f^{n+1/2}). \end{cases}$$

Strang splitting scheme with Crank-Nicolson method

$$
\begin{cases}
(u^{n+1/2}, v) + \dfrac{\tau}{4}\left(\alpha\dfrac{\partial u^{n+1/2}}{\partial x}, \dfrac{\partial v}{\partial x}\right) + \dfrac{\tau}{4}\left(\beta_x\dfrac{\partial u^{n+1/2}}{\partial x}, v\right) = \\
= (u^n, v) - \dfrac{\tau}{4}\left(\alpha\dfrac{\partial u^n}{\partial x}, \dfrac{\partial v}{\partial x}\right) - \dfrac{\tau}{4}\left(\beta_x\dfrac{\partial u^n}{\partial x}, v\right) + \dfrac{\tau}{4}(f^{n+1/2} + f^n, v), \\
\\
(u^{n+1}, v) + \dfrac{\tau}{2}\left(\alpha\dfrac{\partial u^{n+1}}{\partial y}, \dfrac{\partial v}{\partial y}\right) + \dfrac{\tau}{2}\left(\beta_y\dfrac{\partial u^{n+1}}{\partial y}, v\right) = \\
= (u^n, v) - \dfrac{\tau}{2}\left(\alpha\dfrac{\partial u^n}{\partial y}, \dfrac{\partial v}{\partial y}\right) - \dfrac{\tau}{2}\left(\beta_y\dfrac{\partial u^n}{\partial y}, v\right), \\
\\
(u^{n+1}, v) + \dfrac{\tau}{4}\left(\alpha\dfrac{\partial u^{n+1}}{\partial x}, \dfrac{\partial v}{\partial x}\right) + \dfrac{\tau}{4}\left(\beta_x\dfrac{\partial u^{n+1}}{\partial x}, v\right) = \\
= (u^{n+1/2}, v) - \dfrac{\tau}{4}\left(\alpha\dfrac{\partial u^{n+1/2}}{\partial x}, \dfrac{\partial v}{\partial x}\right) - \dfrac{\tau}{4}\left(\beta_x\dfrac{\partial u^{n+1/2}}{\partial x}, v\right) + \dfrac{\tau}{4}(f^{n+1} + f^{n+1/2}
\end{cases}
$$

Strang splitting scheme with Crank-Nicolson method (matrix form)

$$
\begin{cases}
\left[M^x + \frac{\tau}{4}(K^x + G^x)\right] \otimes M^y u^* = \\
\qquad \left[M^x - \frac{\tau}{4}(K^x + G^x)\right] \otimes M^y u^n + \frac{\tau}{4}(F^{n+1/2} + F^n), \\
M^x \otimes \left[M^y + \frac{\tau}{2}(K^y + G^y)\right] u^{**} = M^x \otimes \left[M^y - \frac{\tau}{2}(K^y + G^y)\right] u^*, \\
\left[M^x + \frac{\tau}{4}(K^x + G^x)\right] \otimes M^y u^{n+1} = \\
\qquad \left[M^x - \frac{\tau}{4}(K^x + G^x)\right] \otimes M^y u^{**} + \frac{\tau}{4}(F^{n+1} + F^{n+1/2}).
\end{cases}
$$



Douglas-Gunn scheme for 3D problems

$$\begin{cases} (1 + \frac{\tau}{2}\mathcal{L}_1)u^{n+1/3} = \tau f^{n+1/2} + (1 - \frac{\tau}{2}\mathcal{L}_1 - \tau\mathcal{L}_2 - \tau\mathcal{L}_3)u^n, \\ (1 + \frac{\tau}{2}\mathcal{L}_2)u^{n+2/3} = u^{n+1/3} + \frac{\tau}{2}\mathcal{L}_2 u^n, \\ \quad (1 + \frac{\tau}{2}\mathcal{L}_3)u^{n+1} = u^{n+2/3} + \frac{\tau}{2}\mathcal{L}_3 u^n. \end{cases}$$

Douglas-Gunn scheme for 3D problems

$$
\begin{cases}
(u^{n+1/3}, v) + \dfrac{\tau}{2}\left(\alpha \dfrac{\partial u^{n+1/3}}{\partial x}, \dfrac{\partial v}{\partial x}\right) + \dfrac{\tau}{2}\left(\beta_x \dfrac{\partial u^{n+1/3}}{\partial x}, v\right) = \\
= (u^n, v) - \dfrac{\tau}{2}\left(\alpha \dfrac{\partial u^n}{\partial x}, \dfrac{\partial v}{\partial x}\right) - \dfrac{\tau}{2}\left(\beta_x \dfrac{\partial u^n}{\partial x}, v\right) \\
\qquad - \tau\left(\alpha \dfrac{\partial u^n}{\partial y}, \dfrac{\partial v}{\partial y}\right) - \tau\left(\beta_y \dfrac{\partial u^n}{\partial y}, v\right) \\
\qquad - \tau\left(\alpha \dfrac{\partial u^n}{\partial z}, \dfrac{\partial v}{\partial z}\right) - \tau\left(\beta_z \dfrac{\partial u^n}{\partial z}, v\right) + \tau(f^{n+1/2}, v), \\
(u^{n+2/3}, v) + \dfrac{\tau}{2}\left(\alpha \dfrac{\partial u^{n+2/3}}{\partial y}, \dfrac{\partial v}{\partial y}\right) + \dfrac{\tau}{2}\left(\beta_y \dfrac{\partial u^{n+2/3}}{\partial y}, v\right) = \\
= (u^{n+1/3}, v) + \dfrac{\tau}{2}\left(\alpha \dfrac{\partial u^n}{\partial y}, \dfrac{\partial v}{\partial y}\right) + \dfrac{\tau}{2}\left(\beta_y \dfrac{\partial u^n}{\partial y}, v\right), \\
(u^{n+1}, v) + \dfrac{\tau}{2}\left(\alpha \dfrac{\partial u^{n+1}}{\partial z}, \dfrac{\partial v}{\partial z}\right) + \dfrac{\tau}{2}\left(\beta_z \dfrac{\partial u^{n+1}}{\partial z}, v\right) = \\
= (u^{n+2/3}, v) + \dfrac{\tau}{2}\left(\alpha \dfrac{\partial u^n}{\partial z}, \dfrac{\partial v}{\partial z}\right) + \dfrac{\tau}{2}\left(\beta_z \dfrac{\partial u^n}{\partial z}, v\right),
\end{cases}
$$

Douglas-Gunn scheme for 3D problems

$$
\begin{cases}
\left[M^x + \frac{\tau}{2}(K^x + G^x)\right] \otimes M^y \otimes M^z u^{n+1/3} \\
= \left[M^x - \frac{\tau}{2}(K^x + G^x)\right] \otimes M^y \otimes M^z u^n \\
- \tau M^x \otimes (K^y + G^y) \otimes M^z u^n - \tau M^x \otimes M^y \otimes (K^z + G^z) u^n + \tau F^{n+1/2} \\
M^x \otimes \left[M^y + \frac{\tau}{2}(K^y + G^y)\right] \otimes M^z u^{n+2/3} \\
= M^x \otimes M^y \otimes M^z u^{n+1/3} + M^x \otimes \frac{\tau}{2}(K^y + G^y) \otimes M^z u^n, \\
M^x \otimes M^y \otimes \left[M^z + \frac{\tau}{2}(K^z + G^z)\right] u^{n+1} \\
= M^x \otimes M^y \otimes M^z u^{n+2/3} + M^x \otimes M^y \otimes \frac{\tau}{2}(K^z + G^z) u^n,
\end{cases}
$$

where $M^{x,y,z}$, $K^{x,y,z}$ and $G^{x,y,z}$ are the 1D mass, stiffness and advection matrices, respectively.

Residual minimization method

In all the above methods, in every time step we solve:

$$\text{Find } u \in U \text{ such as } b\left(u,v\right) = l\left(v\right) \quad \forall v \in V, \tag{1}$$

$$b\left(u,v\right) = \left(u,v\right) + dt\left(\left(\beta_i \frac{\partial u}{\partial x_i}, v\right) + \alpha_i\left(\frac{\partial u}{\partial x_i}, \frac{\partial v}{\partial x_i}\right)\right). \tag{2}$$

where $dt = \tau/2$ for the Peaceman-Reachford, $dt = \tau/2$ for the Strang method with backward Euler, and $dt = \tau/4$ for the Strang method with Crank-Nicolson scheme. The right-hand-side $l\left(w,v\right)$ depends on the selected time-integration scheme, e.g. for the Strang method with backward Euler it is

$$l\left(w,v\right) = \left(w + dtf, v\right) \quad \forall v \in V. \tag{3}$$

In our advection-diffusion problem we seek the solution in space

$$U = V = \{v : \int_\Omega \left(v^2 + \frac{\partial v}{\partial x_i}^2\right) < \infty\}. \tag{4}$$

The inner product in V is defined as
$\left(u,v\right)_V = \left(u,v\right)_{L_2} + \left(\frac{\partial u}{\partial x_i}, \frac{\partial v}{\partial x_i}\right)_{L_2}$

Residual minimization method

$$b(u, v) = l(v) \quad \forall v \in V \tag{5}$$

For our weak problem (5) we define the operator $B : U \rightarrow V'$ such as $< Bu, v >_{V' \times V} = b\,(u, v)$.

$$B : U \rightarrow V' \tag{6}$$

such that

$$\langle Bu, v \rangle_{V' \times V} = b(u, v) \tag{7}$$

so we can reformulate the problem as

$$Bu - l = 0 \tag{8}$$

We wish to minimize the residual

$$u_h = argmin_{w_h \in U_h} \frac{1}{2} \| Bw_h - l \|^2_{V'} \tag{9}$$

We introduce the Riesz operator being the isometric isomorphism

$$R_V \colon V \ni v \to (v, .) \in V' \tag{10}$$

We can project the problem back to V

$$u_h = argmin_{w_h \in U_h} \frac{1}{2} \| R_V^{-1}(Bw_h - l) \|_V^2 \tag{11}$$

The minimum is attained at u_h when the Gâteaux derivative is equal to 0 in all directions:

$$\langle R_V^{-1}(Bu_h - l), R_V^{-1}(B\, w_h) \rangle_V = 0 \quad \forall\, w_h \in U_h \tag{12}$$

We define the residual $r = R_V^{-1}(Bu_h - l)$ and we get

$$\langle r, R_V^{-1}(B\, w_h) \rangle = 0 \quad \forall\, w_h \in U_h \tag{13}$$

which is equivalent to

$$\langle Bw_h, r \rangle = 0 \qquad \forall w_h \in U_h. \tag{14}$$

From the definition of the residual we have

$$(r, v)_V = \langle Bu_h - l, v \rangle \quad \forall v \in V. \tag{15}$$

Residual minimization method with semi-infinite problem

Find $(r, u_h)_{V \times U_h}$ such as

$$\begin{aligned} (r, v)_V - \langle Bu_h - l, v \rangle &= 0 \quad \forall v \in V \\ \langle Bw_h, r \rangle &= 0 \quad \forall w_h \in U_h \end{aligned} \tag{16}$$

We discretize the test space $V_m \in V$ to get the discrete problem:
Find $(r_m, u_h)_{V_m \times U_h}$ such as

$$\begin{aligned} (r_m, v_m)_{V_m} - \langle Bu_h - l, v_m \rangle &= 0 \quad \forall v_m \in V_m \\ \langle Bw_h, r_m \rangle &= 0 \quad \forall w_h \in U_h \end{aligned} \tag{17}$$

where $(*, *)_{V_m}$ is an inner product in V_m, $\langle Bu_h, v_m \rangle = b(u_h, v_m)$, $\langle Bw_h, r_m \rangle = b(w_h, r_m)$.

Remark

We define the discrete test space V_m in such a way that it is as close as possible to the abstract V space, to ensure stability, in a sense that the discrete inf-sup condition is satisfied. In our method it is possible to gain stability enriching the test space V_m without changing the trial space U_h.

Discretization of the residual minimization method

We approximate the solution with tensor product of one dimensional B-splines basis functions of order p

$$u_h = \sum_{i,j} u_{i,j} B^x_{i;p}(x) B^y_{j;p}(y). \tag{18}$$

We test with tensor product of one dimensional B-splines basis functions, where we enrich the order in the direction of the x axis from p to r ($r \geq p$, and we enrich the space only in the direction of the alternating splitting)

$$v_m \leftarrow B^x_{i;r}(x) B^y_{j;p}(y). \tag{19}$$

We approximate the residual with tensor product of one dimensional B-splines basis functions of order p

$$r_m = \sum_{s,t} r_{s,t} B^x_{s;r}(x) B^y_{t;p}(y), \tag{20}$$

and we test again with tensor product of 1D B-spline basis functions of order r and p, in the corresponding directions

$$w_h \leftarrow B^x_{k;p}(x) B^y_{l;p}(y). \tag{21}$$

$$A = A_y \otimes A_x ; B = B_x \otimes B_y ; B^T = B_y^T \otimes B_x^T ; A_y = B_y$$

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} = \begin{pmatrix} A_x & B_x \\ B_x^T & 0 \end{pmatrix} \begin{pmatrix} A_y & 0 \\ 0 & A_y^T \end{pmatrix} = \begin{pmatrix} A_x A_y & B_x A_y \\ B_x^T A_y^T & 0 \end{pmatrix}.$$

Both matrices $\begin{pmatrix} A_x & B_x \\ B_x^T & 0 \end{pmatrix}$ and $\begin{pmatrix} A_y & 0 \\ 0 & A_y^T \end{pmatrix}$ can be factorized in a linear $\mathcal{O}(N)$ computational cost.

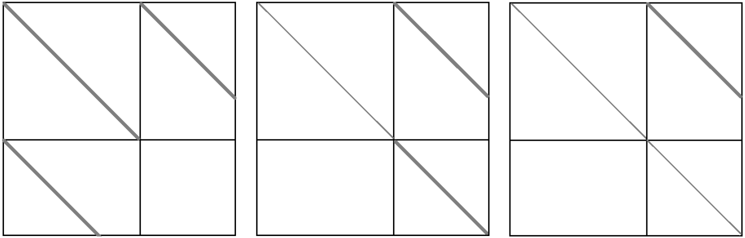


Figure: Factorization of the first sub-matrix.

Numerical results: manufactured solution

Two-dimensional advection-diffusion problem

$$\frac{du}{dt} - \nabla \cdot (K \nabla u) + \beta \cdot \nabla u = f,$$

with $\epsilon = 10^{-2}$, $\beta = (1, 0)$, with zero Dirichlet boundary conditions solved on a square $[0, 1]^2$ domain.
We setup the forcing function $f(x, y, t)$ in such a way that it delivers the manufactured solution of the form $u(x, y, t) = \sin(\Pi x) \sin(\Pi y) \sin(\Pi t)$ on a time interval $[0, 2]$.

Numerical results: manufactured solution

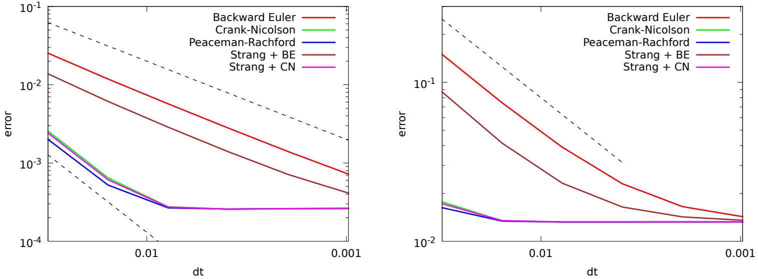


Figure: Convergence in L2 and H1 norms for different time integration schemes on 8×8 mesh.

Numerical results: manufactured solution

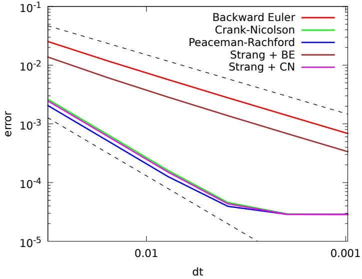


Figure: Convergence in L2 and H1 norms for different time integration schemes on 16×16 mesh.

Numerical results: manufactured solution

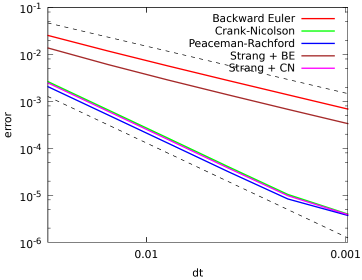


Figure: Convergence in L2 and H1 norms for different time integration schemes on 32×32 mesh.

Two-dimensional numerical results

Propagation of the pollutant from a chimney modeled by the f function, distributed by the wind blowing with changing directions, modeled by β function, and the diffusion phenomena modeled by the coefficients K, over $\Omega = 5000 \times 5000$ meters.

$$\frac{du}{dt} - \nabla \cdot (K \nabla u) + \beta \cdot \nabla u = f$$

$$K = (50, 0.5)$$

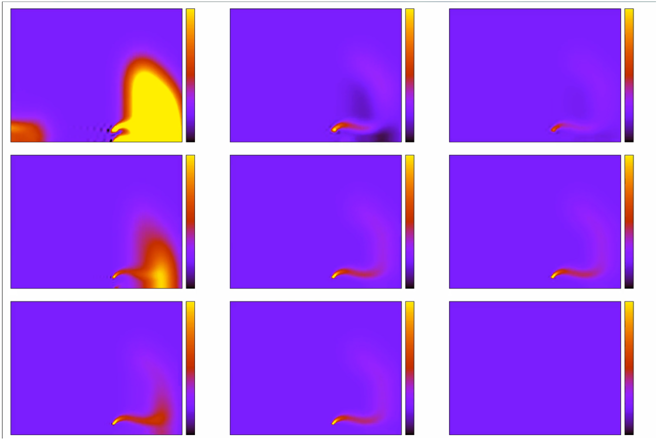
$$\beta = (\beta^x(t), \beta^y(t)) = (\cos a(t), \sin a(t))$$

$$a(t) = \frac{\pi}{3}(\sin(s) + \frac{1}{2}\sin(2.3s)) + \frac{3}{8}\pi$$

$$f(p) = (r-1)^2(r+1)^2$$

where $r = \min(1, (|p - p_0|/25)^2)$, and p represents the distance from the source, and p_0 is the location of the source $p_0 = (3, 2)$.

Numerical results



Trial space: quadratic B-splines
Rows: Mesh size $N = 50, 100, 150$
Columns: Test-space B-splines of order $2 + k$ for $k = 0, 1, 2, 3, 4$
(quadratic C^1, cubics C^2, quartics C^3)

Stationary problems

M. Los, Q.Deng, I. Muga, V.M.Calo, M. Paszynski, Isogeometric Residual Minimization Method (iGRM) with Direction Splitting Preconditoner for Stationary Advection-Diffusion Problems, submitted to *Computer Methods in Applied Mechanics and Engineering* (2019) **IF: 4.441**

Quanling Deng, Ph.D. Curtin University, Perth, Australia

Ignacio Muga, Professor, The Pontifical Catholic University of Valparaiso, Chile

Victor Manuel Calo, Professor, Curtin University, Perth, Australia

Towards iterative solver

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} r \\ u \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix}$$

$$A = M + \eta K$$

$$\begin{aligned} M &= M_x \otimes M_y, \\ K &= K_x \otimes M_y + M_x \otimes K_y. \end{aligned}$$

$$\begin{aligned} A &= M + \eta K \\ &= (M_x + \eta K_x) \otimes (M_y + \eta K_y) - \eta^2 K_x \otimes K_y \\ &= \tilde{A} - \eta^2 \tilde{K} \end{aligned}$$

Towards iterative solver

We start from initial guess $\begin{bmatrix} r^k \\ u^k \end{bmatrix}$, and we compute the update necessary to perform to get the exact solution

$$\begin{bmatrix} d \\ c \end{bmatrix} = \begin{bmatrix} r - r^k \\ u - u^k \end{bmatrix}$$

The update can be obtained by solving

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} r \\ u \end{bmatrix} - \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} r^k \\ u^k \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} d \\ c \end{bmatrix} = \begin{bmatrix} F - Ar^k - Br^k \\ -B^T r^k \end{bmatrix}$$

This is expensive to factorize, so we replace A by approximation $\tilde{A}$

$$\begin{bmatrix} \tilde{A} & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} d \\ c \end{bmatrix} = \begin{bmatrix} F - Ar^k - Br^k \\ -B^T r^k \end{bmatrix}$$

Towards iterative solver

Initialize $\{u^0 = 0; r^0 = 0\}$ **for** $k = 1, ..., N$ until convergence

Compute Schur complement with linear $\mathcal{O}(N)$ cost

$$\begin{bmatrix} \tilde{A} & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} d^k \\ c^k \end{bmatrix} = \begin{bmatrix} F - Ar^k - Br^k \\ -B^T r^k \end{bmatrix}$$

Solve

$$B^T \tilde{A} B u^k = B^T r^k - B^T \tilde{A} F + B^T \tilde{A} A r^k + B^T \tilde{A} B r^k$$

using either MUMPS or PCG

$$r^{k+1} = d^k + r^k$$

$$u^{k+1} = c^k + u^k$$

$$k = k + 1;$$

Algorithm 1: Iterative algorithm

A manufactured solution problem: strong form

We focus on a model problem with a manufactured solution. For a unitary square domain $\Omega = (0,1)^2$, the advection vector $\beta = (1,1)^T$, and $Pe = 100, \epsilon = 1/Pe$ we seek the solution of the advection-diffusion equation

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

with Dirichlet boundary conditions $u = g$ on the whole of $\Gamma = \partial\Omega$. We utilize a manufactured solution

$$u(x,y) = (x + \frac{e^{Pe*x} - 1}{1 - e^{Pe}})(y + \frac{e^{Pe*y} - 1}{1 - e^{Pe}})$$

enforced by the right-hand side, and we use homogeneous Dirichlet boundary conditions on $\partial\Omega$.

A manufactured solution problem: weak form

$$b(u,v) = l(v) \quad \forall v \in V$$

$$\begin{aligned} b(u,v) = &\left(\frac{\partial u}{\partial x}, v\right)_\Omega + \left(\frac{\partial u}{\partial y}, v\right)_\Omega + \epsilon\left(\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}\right)_\Omega + \epsilon\left(\frac{\partial u}{\partial y}, \frac{\partial v}{\partial y}\right)_\Omega \\ &- \left(\epsilon\frac{\partial u}{\partial x} n_x, v\right)_\Gamma - \left(\epsilon\frac{\partial u}{\partial y} n_y, v\right)_\Gamma \\ &- (u, \epsilon\nabla v \cdot n)_\Gamma - (u, \beta \cdot nv)_\Gamma - \left(u, 3p^2\epsilon/hv\right)_\Gamma \end{aligned}$$

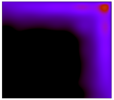
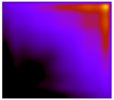
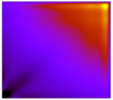
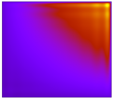
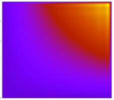
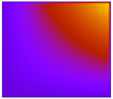
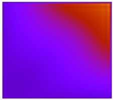
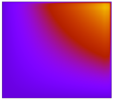
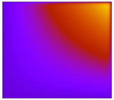
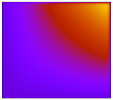
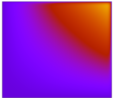
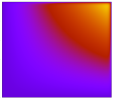
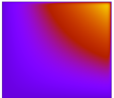
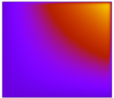
$n = (n_x, n_y)$ is versor normal to Γ, and h is element diameter,

$$l(v) = (f,v)_\Omega - (g, \epsilon\nabla v \cdot n)_\Gamma - (g, \beta \cdot nv)_\Gamma - \left(g, 3p^2\epsilon/hv\right)_\Gamma$$

red terms correspond to weak imposition of the Dirichlet b.c. on Γ with $g = 0$, f is the manufactured solution, blue terms are the integration by parts, gray terms the penalty terms. We seek the solution in space $U = V = H^1(\Omega)$. The inner product in V is

$$(u,v)_V = (u,v)_{L_2} + \left(\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}\right)_{L_2} + \left(\frac{\partial u}{\partial y}, \frac{\partial v}{\partial y}\right)_{L_2}$$

A manufactured solution results

n	trial(2,1) test(2,0)	trial(3,2) test(2,0)	trial(4,3) test(2,0)	trial(5,4) test(2,0)
#DOF L2 H1 8×8	389 192 101 	410 151 74 	433 78 44 	458 28 32 
#DOF L2 H1 16×16	1413 80 59 	1450 16 29 	1489 3.29 18 	1530 1.48 10 
#DOF L2 H1 32×32	5381 32 31 	5450 1.33 9.77 	5521 0.27 3.16 	5594 0.056 0.82 
#DOF L2 H1 64×64	20997 7.66 9.86 	21130 0.07 1.67 	21265 0.01 0.26 	21402 0.003 0.068 

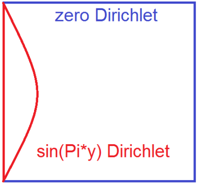
Eriksson-Johnson problem strong form

Given $\Omega = (0,1)^2$, $\beta = (1,0)^T$, we seek the solution of the advection-diffusion problem

$$\frac{\partial u}{\partial x} - \epsilon \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0$$

with Dirichlet boundary conditions

$$u = 0 \text{ for } x \in (0,1), y \in \{0,1\} \qquad u = sin(\Pi y) \text{ for } x = 0$$



The problem is driven by the inflow Dirichlet boundary condition. It develops a boundary layer of width ϵ at the outflow $x = 1$.

We introduce first the weak formulation for the Eriksson-Johnson problem

$$b(u,v) = l(v) \quad \forall v \in V$$

$$b(u,v) = \left(\frac{\partial u}{\partial x}, v\right) + \epsilon\left(\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}\right) + \epsilon\left(\frac{\partial u}{\partial y}, \frac{\partial v}{\partial y}\right)$$
$$-\left(\epsilon\frac{\partial u}{\partial x}n_x, v\right)_\Gamma - \left(\epsilon\frac{\partial u}{\partial y}n_y, v\right)_\Gamma$$
$$-(u, \epsilon\nabla v \cdot n)_\Gamma - (u, \beta \cdot nv)_\Gamma - \left(u, 3p^2\epsilon/hv\right)_\Gamma$$

where the blue, red, and gray terms correspond to the weak imposition of the Dirichlet b.c. on the boundary Γ, and $n = (n_x, n_y)$ is the versor normal to the boundary,

$$l(v) = -(g, \epsilon\nabla v \cdot n)_{\Gamma^-} - (g, \beta \cdot nv)_{\Gamma^-} - \left(g, 3p^2\epsilon/hv\right)_{\Gamma^-} \qquad (22)$$

where the red and gray terms correspond to the weak introduction of the Dirichlet b.c. on the boundary Γ.
We plug the weak form and the inner product into the iGRM setup and we use the preconditioned CG solver.

Residual minimization method for Eriksson-Johnson problem

Find $(r_m, u_h)_{V_m \times U_h}$ such as

$$(r_m, v_m)_{V_m} - \left(\frac{\partial u_h}{\partial x}, v_m\right) - \epsilon\left(\frac{\partial u_h}{\partial x}, \frac{\partial v_m}{\partial x} + \frac{\partial u_h}{\partial y}, \frac{\partial v_m}{\partial y}\right) = (f, v_m) \qquad \forall v_m \in V_m$$

$$\left(\frac{\partial w_h}{\partial x}, r_m\right) + \epsilon\left(\frac{\partial w_h}{\partial x}, \frac{\partial r_m}{\partial x} + \frac{\partial w_h}{\partial y}, \frac{\partial r_m}{\partial y}\right) = 0 \qquad \forall w_h \in U_h$$

where $(r_m, v_m)_{V_m} = (r_m, v_m) + (\frac{\partial r_m}{\partial x}, \frac{\partial v_m}{\partial x}) + (\frac{\partial r_m}{\partial y}, \frac{\partial v_m}{\partial y})$ is the H^1 norm induced inner product.

Remark

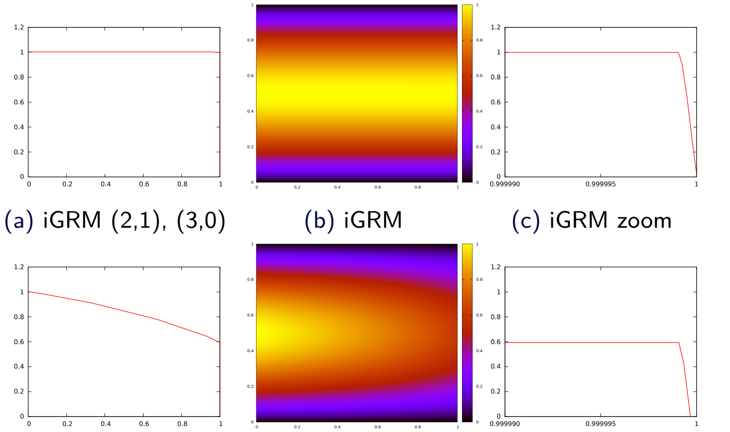
We will use trial space U_h as quadratic B-splines with C^1 continuity and test space V_h as cubic B-splines with C^2 continuity

$$b(u,v) + (R(u), \tau\beta\cdot\nabla v) = l(v) \quad \forall v \in V \tag{23}$$

where $R(u) = \frac{\partial u}{\partial x} + \epsilon\Delta u$, and $\tau^{1/2} = \left(\frac{\beta_x}{h_x} + \frac{\beta_y}{h_y}\right) + 3\epsilon\frac{1}{h_x^2+h_y^2}$, and in our case diffusion term $\epsilon = 10^{-6}$, and convection term $\beta = (1,0)$, and h_x and h_y are dimensions of an element.

$$b_{SUPG}(u,v) = l(v) \quad \forall v \in V \tag{24}$$

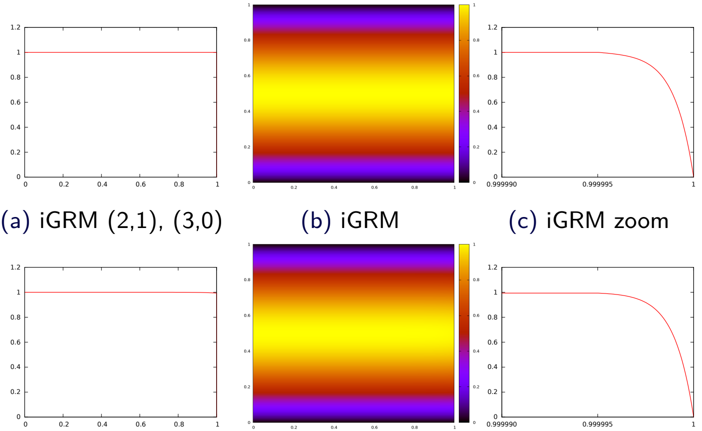
$$\begin{aligned} b_{SUPG}(u,v) = {} & \left(\frac{\partial u}{\partial x}, v\right) + \epsilon\left(\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}\right) + \epsilon\left(\frac{\partial u}{\partial y}, \frac{\partial v}{\partial y}\right) \\ & - \left(\epsilon\frac{\partial u}{\partial x}n_x, v\right)_\Gamma - \left(\epsilon\frac{\partial u}{\partial y}n_y, v\right)_\Gamma \\ & - (u, \epsilon\nabla v\cdot n)_\Gamma - (u, \beta\cdot nv)_\Gamma - \left(u, 3p^2\epsilon/hv\right)_\Gamma \\ & + \left(\frac{\partial u}{\partial x} + \epsilon\Delta u, \left(\frac{1}{h_x} + 3\epsilon\frac{1}{h_x^2+h_y^2}\right)^2\frac{\partial v}{\partial x}\right) \end{aligned}$$



(a) iGRM (2,1), (3,0) (b) iGRM (c) iGRM zoom

(d) SUPG trial (3,2) (e) SUPG (f) SUPG zoom

Figure: Comparison of solutions of the Erikkson-Johnsson by using iGRM and SUPG methods for Pe=1,000,000 on 2x2 mesh,
using (2,1) for trial and (3,0) for testing.



(a) iGRM (2,1), (3,0)   (b) iGRM   (c) iGRM zoom

(d) SUPG trial (3,2)   (e) SUPG   (f) SUPG zoom

Figure: Comparison of solutions of the Erikkson-Johnsson by using iGRM and SUPG methods for Pe=1,000,000 on 32x32 mesh, using (2,1) for trial and (3,0) for testing.

Circular wind problem

$$\beta_x \frac{\partial u}{\partial x} + \beta_y \frac{\partial u}{\partial y} - \epsilon \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0$$

over the rectangular domain $\Omega = (0,1) \times (-1,1)$, with zero right-hand side $f = 0$, $Pe = 1,000,000$, the advection vector $\beta(x,y) = (\beta_x(x,y), \beta_y(x,y)) = \psi(\frac{-y}{(x^2+y^2)^{\frac{1}{2}}}, \frac{x}{(x^2+y^2)^{\frac{1}{2}}})$ modeling the circular wind, where ψ is the wind force coefficient.

$\Gamma_1 = \{(x,y) : x = 0, 0.5 \leq y \leq 1.0\}$,
$\Gamma_2 = \{(x,y) : x = 0, 0.0 \leq y \leq 0.5\}$,
$\Gamma_3 = \{(x,y) : x = 0, -0.5 \leq y \leq 0.0\}$,
$\Gamma_4 = \{(x,y) : x = 0, -1.0 \leq y \leq -0.5\}$,
We utilize the Dirichlet boundary conditions $u = g$ on $\Gamma = \partial\Omega$ where

$$g = \frac{1}{2}\left(\tanh\left((|y| - 0.35)\frac{b}{\epsilon}\right) + 1\right), \text{ for } x \in \Gamma_2 \cup \Gamma_3$$

$$g = \frac{1}{2}\left(0.65 - \tanh\left((|y|)\frac{b}{\epsilon}\right) + 1\right), \text{ for } x \in \Gamma_1 \cup \Gamma_4$$

$$g = 0, \text{ for } x \in \Gamma \setminus \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$$

Circular wind problem

The weak formulation

$$b(u,v) = l(v) \quad \forall v \in V$$

$$\begin{aligned} b(u,v) = \\ \left(\beta_x \frac{\partial u}{\partial x}, v\right)_\Omega + \left(\beta_y \frac{\partial u}{\partial y}, v\right)_\Omega + \epsilon \left(\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}\right)_\Omega + \epsilon \left(\frac{\partial u}{\partial y}, \frac{\partial v}{\partial y}\right)_\Omega \\ - \left(\epsilon \frac{\partial u}{\partial x} n_x, v\right)_\Gamma - \left(\epsilon \frac{\partial u}{\partial y} n_y, v\right)_\Gamma \\ - (u, \epsilon \nabla v \cdot n)_\Gamma - (u, \beta \cdot n v)_\Gamma - \left(u, 3p^2 \epsilon / h v\right)_\Gamma \end{aligned}$$

where $n = (n_x, n_y)$ is the versor normal to Γ,

$$l(v) = -(g, \epsilon \nabla v \cdot n)_\Gamma - (g, \beta \cdot n v)_\Gamma - \left(g, 3p^2 \epsilon / h v\right)_\Gamma$$

$n = (n_x, n_y)$ is the versor normal to the boundary, and the right-hand side forcing is equal to 0.

Circular wind problem

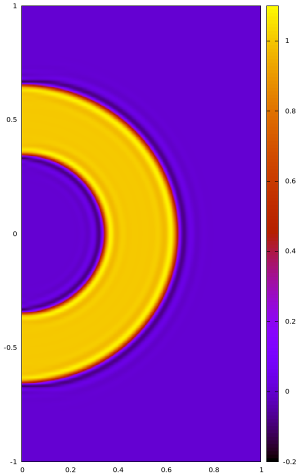


Figure: Solution to the circular wind problem on the mesh of 128×128 elements with trial(2,1),test(2,0), for Pecklet number $Pe = 1,000,000$, wind force $b = 1$. Horizontal cross-section at $x = 0$.

Conclusions

- **isoGeometric Residual Minimization Method (iGRM)** for time-dependent problems
  - 2^{nd} order time schemes (unconditional stability in time)
  - Residual minimization for each time step (stability in space)
  - Discretization with B-spline basis functions (higher continuity smooth solutions)
  - Kronecker product structure of the matrix (linear cost $\mathcal{O}(N)$ of direct solver)
- **isoGeometric Residual Minimization Method (iGRM)** for stationary problems
  - Residual minimization (stability in space)
  - Discretization with B-spline basis functions (higher continuity smooth solutions)
  - Kronecker product structure of the inner product matrix (linear cost $\mathcal{O}(N)$ preconditioner for iterative solver)
  - Symmetric positive definite system (convergence of the conjugated gradient method)
- **IGA-ADS** `https://github.com/marcinlos/iga-ads`

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