Virtual Element approximation of non-newtonian fluids

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Joint work with:
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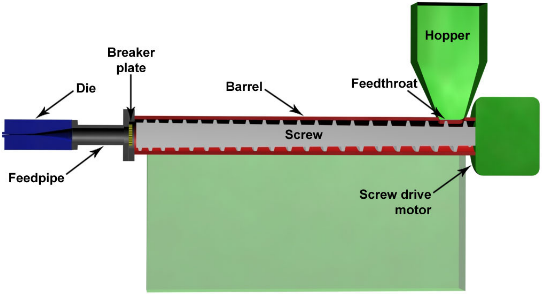
Outline

Motivation: Extrusion



Extrusion is the process of turning materials (e.g. rubber) into a specifically shaped product.

- From the hopper, the stock is sent to the barrel where it is softened through heating and shearing and pressurised by the screw's rotation process.
- The pressurised stock is pushed into the die (with a particular cross section) and as it emerges it acquires its shape.

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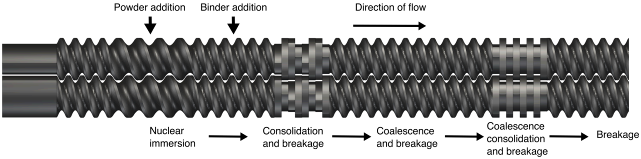

Example of a Twin-Screw Extruder

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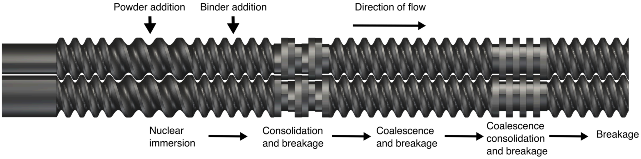

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Key aspects of the numerical simulation of the extrusion process:

- complex and moving geometry;
- non-newtonian rheology;
- data driven rheological constitutive law.

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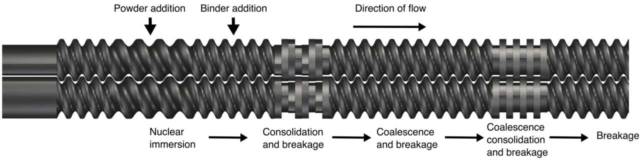

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VEM

Neural Networks

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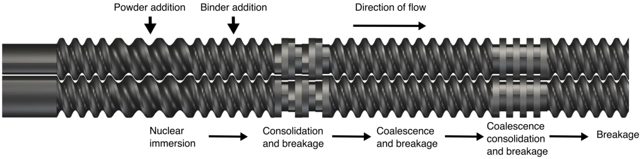

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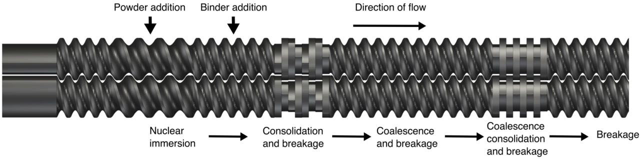

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VEM ⇝ **Neural Networks**

[Parolini, Poiatti, Vené, V. , arXiv:2401.07121]

Very short VEM literature overview for flow problems

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  [Beirão da Veiga, Lovadina, Vacca, 2017 & 2018], $\cdots$

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\begin{aligned}
-\mathbf{div}(\nu(\vartheta)\,\boldsymbol{\varepsilon}(\boldsymbol{u})) + (\boldsymbol{\nabla}\boldsymbol{u})\,\boldsymbol{u} - \nabla p &= \boldsymbol{f} && \text{in } \Omega,\\
\operatorname{div}\boldsymbol{u} &= 0 && \text{in } \Omega,\\
-\operatorname{div}(\kappa\,\nabla\vartheta) + \boldsymbol{u}\cdot\nabla\vartheta &= g && \text{in } \Omega,\\
\boldsymbol{u} &= 0 && \text{on } \partial\Omega,\\
\vartheta &= \vartheta_{\mathrm{D}} && \text{on } \partial\Omega.
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[Antonietti, Vacca, V. Virtual element method for the Navier–Stokes equation coupled with the heat equation, IMAJNA, 2022]

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- VEM for non-Newtonian Stokes (this Talk)
  [Antonietti, Beirao da Veiga, Botti, Vacca, V. A Virtual Element method for non-Newtonian pseudoplastic Stokes flows, CMAME, 2024]

Very incomplete literature overview

FEM: Baranger, Najib, 1990; Sandri 1993; Barrett, Liu, 1994; Belenki, Berselli, Diening, Ruzicka, 2012; Hirn, 2013; Kreuzer,Süli, 2016; Kaltenbach, Ruzicka, 2023; ...

HHO: Botti, Castanon Quiroz, Di Pietro, Harnist,2021; Castanon Quiroz, Di Pietro, and A. Harnist, 2021; ...

...

Non-Newtonian Stokes flow: continuous problem

$$
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-\nabla \cdot \boldsymbol{\sigma}(\varepsilon(\mathbf{u})) + \nabla \mathbf{p} &= \mathbf{f} && \text{in } \boldsymbol{\Omega}, \\
\nabla \cdot \mathbf{u} &= 0 && \text{in } \Omega, \\
\mathbf{u} &= \mathbf{0} && \text{on } \boldsymbol{\Gamma},
\end{aligned}
$$

with

$$
\boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\boldsymbol{v})) = \underbrace{(\delta^2 + |\boldsymbol{\varepsilon}(\boldsymbol{v})|^2)^{\frac{r-2}{2}}}_{\kappa(|\boldsymbol{\varepsilon}(\boldsymbol{v})|)} \boldsymbol{\varepsilon}(\boldsymbol{v}), \quad r \in (1, 2]
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and $\delta \geq 0$.

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and $\delta \geq 0$.

Viscosity κ depends on shear rate. (for $r = 2$ newtonian fluids).

Weak formulation

Set

$$\boldsymbol{V} = \boldsymbol{W}_0^{1,r}(\Omega) \qquad Q = \left\{ q \in L^{r'}(\Omega) \ : \ \textstyle\int_\Omega q = 0 \right\}$$

Let $\boldsymbol{f} \in \boldsymbol{L}^{r'}(\Omega)$, find $(\boldsymbol{u}, p) \in \boldsymbol{V} \times Q$ s. t.

$$\begin{aligned} a(\boldsymbol{u}, \boldsymbol{v}) + b(\boldsymbol{v}, p) &= \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v} \qquad && \forall \boldsymbol{v} \in \boldsymbol{V}, \\ -b(\boldsymbol{u}, q) &= 0 && \forall q \in P, \end{aligned}$$

where

$$a(\boldsymbol{w}, \boldsymbol{v}) := \int_\Omega \boldsymbol{\sigma}(\varepsilon(\boldsymbol{w})) : \varepsilon(\boldsymbol{v}), \qquad b(\boldsymbol{v}, q) := -\int_\Omega (\nabla \cdot \boldsymbol{v}) q.$$

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$\rightsquigarrow$ the problem is well-posed in $\boldsymbol{V} \times P$ [Barrett, Liu, 1994]

Virtual space of velocities and pressures

We consider on each polygonal element $E \in \Omega_h$ the "enhanced" virtual space

$$\boldsymbol{V}_h(E) := \Big\{ \boldsymbol{v}_h \in [C^0(\overline{E})]^2 :$$

$$\begin{aligned} &(i)\ \boldsymbol{\Delta} \boldsymbol{v}_h + \nabla s \in \boldsymbol{x}^\perp \mathbb{P}_{k-1}(E), \quad \text{for some } s \in L^2_0(E), \\ &(ii)\ \operatorname{div} \boldsymbol{v}_h \in \mathbb{P}_{k-1}(E)\,, \\ &(iii)\ \boldsymbol{v}_{h|e} \in [\mathbb{P}_k(e)]^2 \ \ \forall e \in \partial E, \\ &(iv)\,(\boldsymbol{v}_h - \Pi_k^{\nabla,E} \boldsymbol{v}_h,\, \boldsymbol{x}^\perp\, \widehat{p}_{k-1})_E = 0 \ \ \forall \widehat{p}_{k-1} \in \widehat{\mathbb{P}}_{k-1\backslash k-3}(E) \end{aligned} \Big\}$$

where $\boldsymbol{x}^\perp = (x_2, -x_1)$.

See [Beirão da Veiga, Lovadina, Vacca, 2017&2018]

(P1) Polynomial inclusion: $[\mathbb{P}_k(E)]^2 \subseteq \boldsymbol{V}_h(E)$;

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(P2) Degrees of freedom:

$\mathbf{D_V}$1 values of $\boldsymbol{v}_h$ at the vertexes of the polygon E,

$\mathbf{D_V}$2 values of $\boldsymbol{v}_h$ at $k-1$ distinct points of every edge $e \in \partial E$,

$\mathbf{D_V}$3 moments of $\boldsymbol{v}_h$

$$\frac{1}{|E|}\int_E \boldsymbol{v}_h \cdot \boldsymbol{m}^{\perp} m_{\boldsymbol{\alpha}} \,\mathrm{d}E \qquad \text{for any } m_{\boldsymbol{\alpha}} \in \mathbb{M}_{k-3}(E),$$

where $\boldsymbol{m}^{\perp} := \frac{1}{h_E}(x_2 - x_{2,E}, -x_1 + x_{1,E})$,

$\mathbf{D_V}$4 the moments of $\mathrm{div}\,\boldsymbol{v}_h$

$$\frac{h_E}{|E|}\int_E \mathrm{div}\,\boldsymbol{v}_h \, m_{\boldsymbol{\alpha}} \,\mathrm{d}E \qquad \text{for any } m_{\boldsymbol{\alpha}} \in \mathbb{M}_{k-1}(E) \text{ with } |\boldsymbol{\alpha}| > 0;$$

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(P3) Polynomial projections: the DoFs $\mathbf{D}_{\boldsymbol{V}}$ allow us to compute the following linear operators:

$$\Pi_k^{0,E} \colon \boldsymbol{V}_h(E) \to [\mathbb{P}_k(E)]^2, \qquad \boldsymbol{\Pi}_{k-1}^{0,E} \colon \boldsymbol{\nabla} \boldsymbol{V}_h(E) \to [\mathbb{P}_{k-1}(E)]^{2\times 2}.$$

Global discrete velocity space $\boldsymbol{V}_h$:

$$\boldsymbol{V}_h := \{\boldsymbol{v}_h \in \boldsymbol{V} \quad \text{s.t.} \quad \boldsymbol{v}_{h|E} \in \boldsymbol{V}_h(E) \quad \text{for all } E \in \Omega_h\}\,.$$

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Discrete inf-sup: for any $r \in (1, 2]$ it exists a constant $\overline{\beta}(r)$, such that

$$\inf_{q_h \in Q_h} \sup_{\boldsymbol{w}_h \in \boldsymbol{V}_h} \frac{b(\boldsymbol{w}_h, q_h)}{\|q_h\|_{L^{r'}(\Omega)} \|\boldsymbol{w}_h\|_{\boldsymbol{W}^{1,r}(\Omega)}} \geq \overline{\beta}(r) > 0.$$

Divergence-free

Let us introduce the discrete kernel

$$\boldsymbol{Z}_h := \{\boldsymbol{v}_h \in \boldsymbol{V}_h \quad \text{s.t.} \quad b(\boldsymbol{v}_h, q_h) = 0 \quad \text{for all } q_h \in Q_h\}$$

then the following kernel inclusion holds

$$\boldsymbol{Z}_h \subseteq \boldsymbol{Z} := \{\boldsymbol{v} \in \boldsymbol{U} \quad \text{s.t.} \quad \nabla\cdot\boldsymbol{v} = 0\},$$

i.e. the functions in the discrete kernel are exactly divergence-free

Discrete forms

$$a_h^E(\boldsymbol{w}_h, \boldsymbol{v}_h) = \int_E \boldsymbol{\sigma}(\boldsymbol{\Pi}_{k-1}^{0,E}\varepsilon(\boldsymbol{w}_h)) : \boldsymbol{\Pi}_{k-1}^{0,E}\varepsilon(\boldsymbol{v}_h) + S^E((I - \Pi_k^{0,E})\boldsymbol{w}_h, (I - \Pi_k^{0,E})\boldsymbol{v}_h)$$

with

$$S^E(\boldsymbol{v}_h, \boldsymbol{w}_h) = h_E^{2-r} \sum_{i=1}^{N_E} |\chi_i(\boldsymbol{v}_h)|^{r-2}\chi_i(\boldsymbol{v}_h)\chi_i(\boldsymbol{w}_h)$$

Properties of Discrete Forms (I)

Let $\boldsymbol{e}_h = \boldsymbol{u}_h - \boldsymbol{w}_h$. For $\Pi_k^{0,E}\boldsymbol{u}_h = \Pi_k^{0,E}\boldsymbol{w}_h = \Pi_k^{0,E}\boldsymbol{v}_h = \boldsymbol{0}$ there hold

- Norm Equivalence:

$$S^E(\boldsymbol{u}_h, \boldsymbol{u}_h) \simeq \|\varepsilon(\boldsymbol{u}_h)\|^r_{\mathbb{L}^r(E)}$$

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- Strong Monotonicity:

$$S^E(\boldsymbol{u}_h, \boldsymbol{e}_h) - S^E(\boldsymbol{w}_h, \boldsymbol{e}_h) \gtrsim \|\varepsilon(\boldsymbol{e}_h)\|_{\mathbb{L}^r(E)}^2 \left(\|\varepsilon(\boldsymbol{u}_h)\|_{\mathbb{L}^r(E)}^r + \|\varepsilon(\boldsymbol{w}_h)\|_{\mathbb{L}^r(E)}^r\right)^{\frac{r-2}{r}}$$

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- Hölder Continuity:

$$|S^E(\boldsymbol{u}_h, \boldsymbol{v}_h) - S^E(\boldsymbol{w}_h, \boldsymbol{v}_h)| \lesssim \|\boldsymbol{e}_h\|^{r-1}_{\boldsymbol{W}^{1,r}(E)} \|\boldsymbol{v}_h\|_{\boldsymbol{W}^{1,r}(E)}$$

Properties of Discrete Forms (II)

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VEM problem

Find $(\boldsymbol{u}_h, p_h) \in \boldsymbol{V}_h \times Q_h$ such that

$$\begin{aligned} a_h(\boldsymbol{u}_h, \boldsymbol{v}_h) + b(\boldsymbol{v}_h, p_h) &= \int_\Omega \boldsymbol{f}_h \cdot \boldsymbol{v}_h \qquad && \forall \boldsymbol{v}_h \in \boldsymbol{V}_h, \\ -b(\boldsymbol{u}_h, q_h) &= 0 && \forall q_h \in Q_h \,. \end{aligned}$$

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\end{aligned}
$$

$\rightsquigarrow$ the discrete problem is well-posed

Equivalently: find $\boldsymbol{u}_h \in \boldsymbol{Z_h}$ such that

$$
a_h(\boldsymbol{u}_h, \boldsymbol{v}_h) = \int_\Omega \boldsymbol{f}_h \cdot \boldsymbol{v}_h \qquad \forall \boldsymbol{v}_h \in \boldsymbol{Z_h}\,.
$$

Error estimates

Theorem [Antonietti, Beirão da Veiga, Botti, Vacca, V., CMAME 2024]

For $\delta = 0$ and sufficiently regular solution $(\boldsymbol{u}, p)$ there holds:

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{W^{1,r}(\Omega)} \lesssim h^{kr/2}$$
$$\|p - p_h\|_{L^{r'}(\Omega)} \lesssim h^{k(r-1)}$$

Recall: $\boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\boldsymbol{v})) = (\delta^2 + |\boldsymbol{\varepsilon}(\boldsymbol{v})|^2)^{\frac{r-2}{2}} \boldsymbol{\varepsilon}(\boldsymbol{v}))$

cf. [Barrett, Liu, 1994]

Proof: Idea

For $\boldsymbol{\xi}_h = \boldsymbol{u}_h - \boldsymbol{u}_I$ we have

$$
\begin{aligned}
& a_h(\boldsymbol{u}_h, \boldsymbol{\xi}_h) - a_h(\boldsymbol{u}_I, \boldsymbol{\xi}_h) = a(\boldsymbol{u}, \boldsymbol{\xi}_h) - a_h(\boldsymbol{u}_I, \boldsymbol{\xi}_h) + (\boldsymbol{f}_h - \boldsymbol{f}, \boldsymbol{\xi}_h) \\
& = \left(\int_\Omega \boldsymbol{\sigma}(\cdot, \varepsilon(\boldsymbol{u})) : \varepsilon(\boldsymbol{\xi}_h) - \int_\Omega \boldsymbol{\sigma}(\cdot, \boldsymbol{\Pi}^0_{k-1}\varepsilon(\boldsymbol{u}_I)) : \boldsymbol{\Pi}^0_{k-1}\varepsilon(\boldsymbol{\xi}_h) \right) - S(\widetilde{\boldsymbol{u}}_I, \widetilde{\boldsymbol{\xi}}_h) \\
& \qquad + (\boldsymbol{f}_h - \boldsymbol{f}, \boldsymbol{\xi}_h) \\
& =: T_1 + T_2 + T_3
\end{aligned}
$$

- Estimate T_1, T_2, T_3
- Use Strong Monotonicity on the left hand-side

Numerical results: Fixed Point Iteration

Notation:

$$\boldsymbol{\sigma}_r(\boldsymbol{x}, \varepsilon(\boldsymbol{z}); \varepsilon(\boldsymbol{v})) := (\delta^2 + |\varepsilon(\boldsymbol{z})|^2)^{\frac{r-2}{2}} \varepsilon(\boldsymbol{v}) \qquad \text{for all } \boldsymbol{z},\ \boldsymbol{v} \in \boldsymbol{V},$$

$$a_r(\boldsymbol{z}; \boldsymbol{v}, \boldsymbol{w}) := \int_\Omega \boldsymbol{\sigma}_r(\cdot, \varepsilon(\boldsymbol{z}); \varepsilon(\boldsymbol{v})) : \varepsilon(\boldsymbol{w}) \qquad \text{for all } \boldsymbol{z},\ \boldsymbol{v},\ \boldsymbol{w} \in \boldsymbol{V},$$

Nonlinear problem

find $(\boldsymbol{u}_h, p_h) \in \boldsymbol{V}_h \times Q_h$ such that

$$a_{r,h}(\boldsymbol{u}_h; \boldsymbol{u}_h, \boldsymbol{v}_h) + b(\boldsymbol{v}_h, p_h) = \int_\Omega \boldsymbol{f}_h \cdot \boldsymbol{v}_h \qquad \forall \boldsymbol{v}_h \in \boldsymbol{V}_h,$$

$$-b(\boldsymbol{u}_h, q_h) = 0 \qquad \forall q_h \in Q_h\,.$$

Numerical results: Fixed Point Iteration

STEP 1. Let $(\boldsymbol{u}_h^{\mathrm{S}}, p_h^{\mathrm{S}})$ be the solution of the linear Stokes equation
Let $\bar{r} := \frac{r+2}{2}$. Starting from $(\boldsymbol{u}_h^0, p_h^0) = (\boldsymbol{u}_h^{\mathrm{S}}, p_h^{\mathrm{S}})$, for $n \geq 0$, until convergence solve

$$
\begin{aligned}
a_{\bar{r},h}(\boldsymbol{u}_h^n; \boldsymbol{u}_h^{n+1}, \boldsymbol{v}_h) + b(\boldsymbol{v}_h, p_h^{n+1}) &= \int_\Omega \boldsymbol{f}_h \cdot \boldsymbol{v}_h \qquad && \forall \boldsymbol{v}_h \in \boldsymbol{V}_h, \\
-b(\boldsymbol{u}_h^{n+1}, q_h) &= 0 && \forall q_h \in Q_h .
\end{aligned}
$$

STEP 2. Let $(\boldsymbol{u}_h^{\bar{r}}, p_h^{\bar{r}})$ be the solution obtained in STEP 1.
Starting from $(\boldsymbol{u}_h^0, p_h^0) = (\boldsymbol{u}_h^{\bar{r}}, p_h^{\bar{r}})$, for $n \geq 0$, until convergence solve

$$
\begin{aligned}
a_{r,h}(\boldsymbol{u}_h^n; \boldsymbol{u}_h^{n+1}, \boldsymbol{v}_h) + b(\boldsymbol{v}_h, p_h^{n+1}) &= \int_\Omega \boldsymbol{f}_h \cdot \boldsymbol{v}_h \qquad && \forall \boldsymbol{v}_h \in \boldsymbol{V}_h, \\
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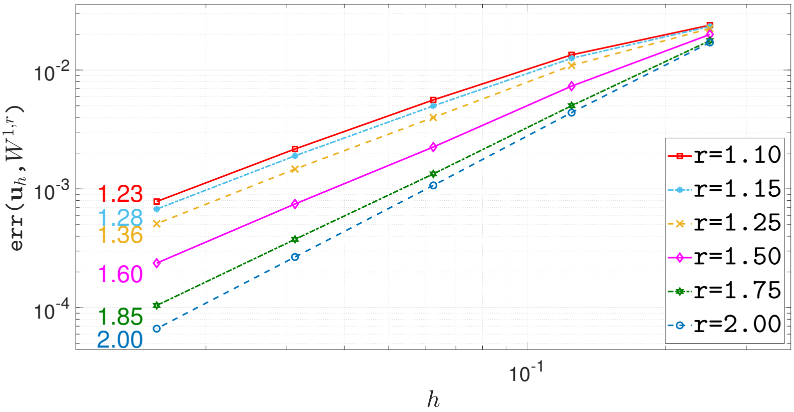
\end{aligned}
$$

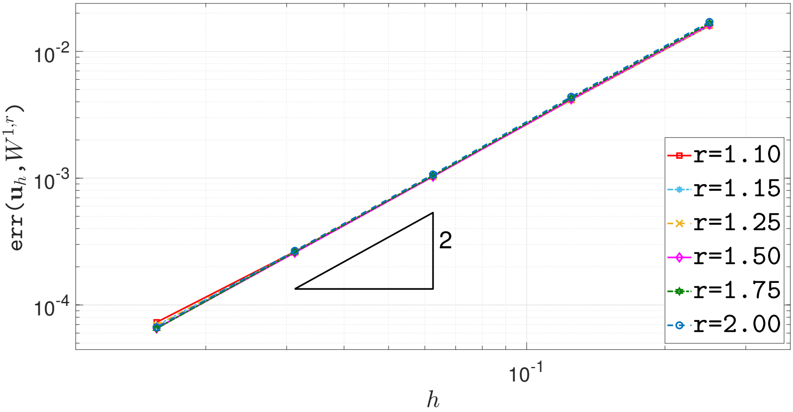
Numerical results: manufactured solution ($k = 2$)



$\delta = 0$

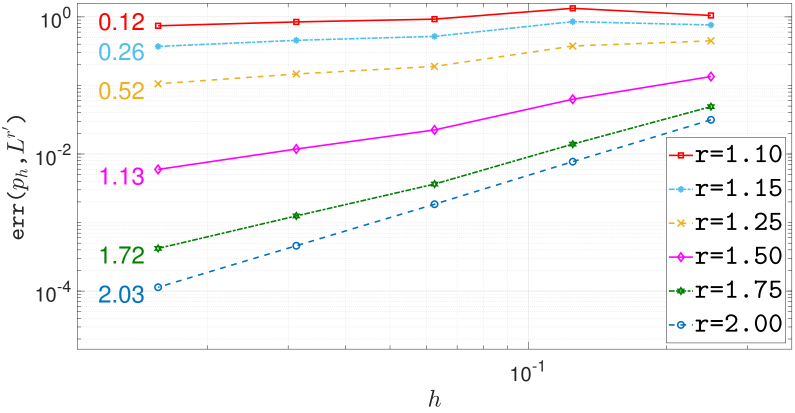
Expected order for velocity: r

Recall: $\boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\boldsymbol{v})) = (\delta^2 + |\boldsymbol{\varepsilon}(\boldsymbol{v})|^2)^{\frac{r-2}{2}} \boldsymbol{\varepsilon}(\boldsymbol{v}))$



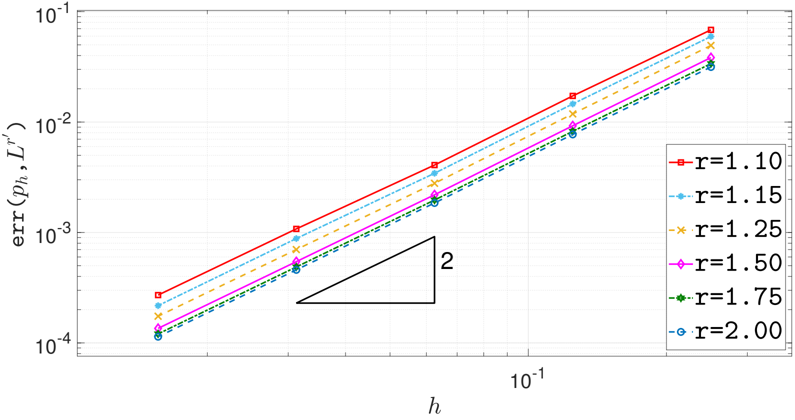
$\delta = 1$

Expected order for velocity: 2 (not covered by theory)



$\delta = 0$

Expected order for pressure: $2(r-1)$



$\delta = 1$

Expected order for pressure: 2 (not covered by theory)

Conclusions and perspectives

We explored:

- VEM for non-Newtonian Stokes flows;

Future work:

- Moving geometries;
- Non-Newtonian laws depending on temperature;
- Combine VEM and Neural Network data driven rheological laws employing [Parolini, Poiatti, Vené, V. , Structure-preserving neural networks in data-driven rheological models, arXiv: 2401.07121, 2024].

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Extra Material (I)

Theorem [Antonietti, Beirão da Veiga, Botti, Vacca, V., CMAME 2024]

Assume that $\boldsymbol{u} \in \boldsymbol{W}^{k_1+1,r}(\Omega_h)$, $\boldsymbol{\sigma}(\cdot, \varepsilon(\boldsymbol{u})) \in \mathbb{W}^{k_2,r'}(\Omega_h)$ and $\boldsymbol{f} \in \boldsymbol{W}^{k_3+1,r'}(\Omega_h)$ for some k_1, k_2, $k_3 \leq k$. Then, we have

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{\boldsymbol{W}^{1,r}(\Omega_h)} \lesssim h^{k_1 r/2} R_1^{r/2} + h^{k_1} R_1 + h^{k_2} R_2 + h^{k_3+2} R_3 \,,$$

where the hidden constant depends on data and the regularity terms are

$$R_1 := |\boldsymbol{u}|_{\boldsymbol{W}^{k_1+1,r}(\Omega_h)} \,, \quad R_2 := |\boldsymbol{\sigma}(\cdot, \varepsilon(\boldsymbol{u}))|_{\mathbb{W}^{k_2,r'}(\Omega_h)} \,, \quad R_3 := |\boldsymbol{f}|_{\boldsymbol{W}^{k_3+1,r'}(\Omega_h)} \,.$$

Extra Material (II)

$$\boldsymbol{u}_{\mathrm{ex}}(x_1, x_2) = |\boldsymbol{x}|^{0.01} \begin{bmatrix} x_2 \\ -x_1 \end{bmatrix}, \qquad p_{\mathrm{ex}}(x_1, x_2) = -|\boldsymbol{x}|^{\gamma} + c_{\gamma}\,.$$

where $\gamma = \frac{2}{r} - 1 + 0.01$ and c_γ is s.t. p_{ex} is zero averaged. Notice that for all $r \in (1, 2]$

$$\boldsymbol{u}_{\mathrm{ex}} \in \boldsymbol{W}^{2/r+1,r}(\Omega)\,, \quad \boldsymbol{\sigma}(\cdot, \varepsilon(\boldsymbol{u}_{\mathrm{ex}})) \in \mathbb{W}^{2/r',r'}(\Omega)$$

$$\boldsymbol{f} \in \boldsymbol{W}^{2/r'-1,r'}(\Omega)\,, \quad p_{\mathrm{ex}} \in W^{1,r'}(\Omega)\,,$$

1/h	r 1.25	1.33	1.50	1.67	1.75	2.00
2	7.51e-04	7.72e-04	8.22e-04	8.73e-04	8.99e-04	9.98e-04
4	2.87e-04	3.03e-04	3.44e-04	3.89e-04	4.13e-04	4.99e-04
8	1.16e-04	1.21e-04	1.42e-04	1.71e-04	1.87e-04	2.48e-04
16	7.47e-05	5.96e-05	6.15e-05	7.50e-05	8.48e-05	1.23e-04
eoc	1.10e+00	1.23e+00	1.24e+00	1.18e+00	1.13e+00	1.00e+00
$\frac{2}{r'}$	0.40	0.50	0.66	0.80	0.86	1.00

Table: Test 2. Errors $\mathtt{err}(\boldsymbol{u}_h, W^{1,r})$.

1/h	r 1.25	1.33	1.50	1.67	1.75	2.00
2	1.21e-01	1.06e-01	9.69e-02	9.97e-02	1.03e-01	1.75e-01
4	8.75e-02	6.78e-02	5.23e-02	5.06e-02	5.17e-02	8.78e-02
8	6.49e-02	4.54e-02	2.90e-02	2.58e-02	2.60e-02	4.37e-02
16	4.87e-02	3.11e-02	1.66e-02	1.32e-02	1.31e-02	2.17e-02
eoc	4.37e-01	5.88e-01	8.48e-01	9.70e-01	9.90e-01	1.00e+00
$\frac{2}{r'}$	0.40	0.50	0.66	0.80	0.86	1.00

Table: Test 2. Errors $\mathtt{err}(p_h, L^{r'})$.