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Anisotropic adaptive finite elments for aluminium electrolysis

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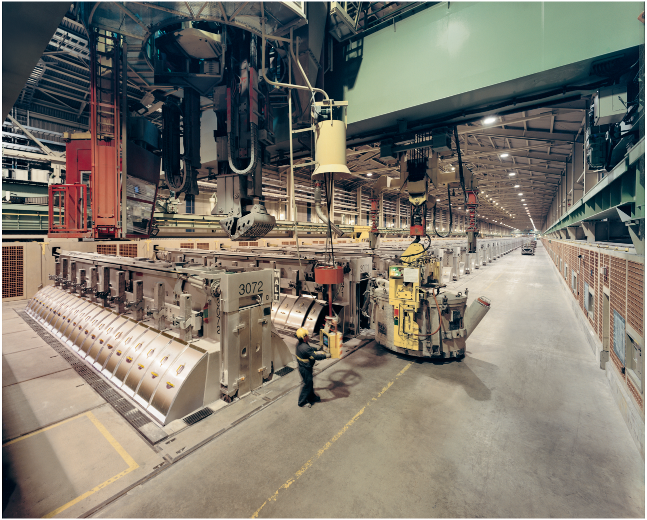
This work is financially supported by Rio Tinto-Aluminium (LRF, Saint-Jean de Maurienne)

Industry of aluminium



Aluminium cells.
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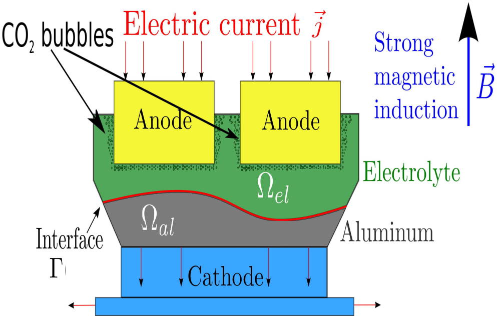
Aluminium electrolysis

- $2Al_2O_3 + 3C \rightarrow 4Al + 3CO_2$



Schema profile view of a cell

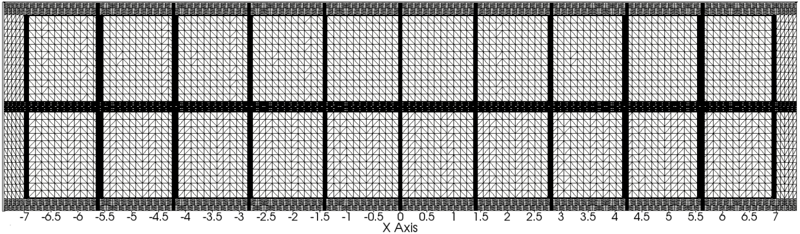
- Difficulties: multi-scale features

Objective of the work

We are mainly concerned on the fluid flow problem of aluminium electrolysis

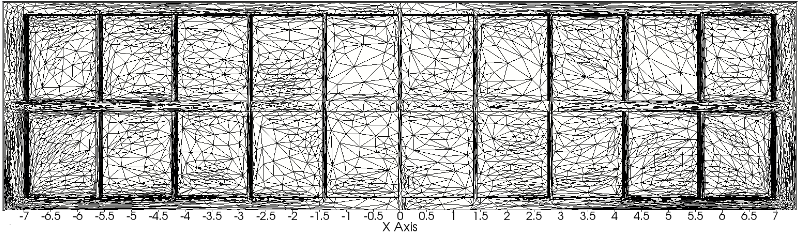
- Goal: Compute velocity by finite elements method for a given precision
- Approach: construct a "better" mesh
- Outcome: a mesh giving a solution with a given precision and with reduced amount of vertices and therefore CPU time
- The anisotropic mesh are produced using the MeshGems commercial software (3D Precise Mesh)

Example of "standard" mesh



- View from above
- 326099 Vertices

Example of adapted mesh (same precision than standard mesh)



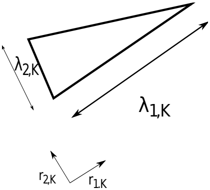
- View from above
- 41687 Vertices

Two model problems

- Let $\Omega \subset \mathbb{R}^2$ and $u : \Omega \to \mathbb{R}$ solution of $-\nabla \cdot (\mu \nabla u) = f$ with zero Dirichlet boundary conditions.
- We consider two different models:
  - Linear: $\mu \in L^\infty(\Omega)$, $0 < \mu_{\min} \leq \mu \leq \mu_{\max}$.
  - Nonlinear: $\mu = \mu_0 + |\nabla u|^{p-2}$, $\mu_0 \geq 0$, $p \geq 3$.
- For any $h > 0$, let $\mathcal{T}_h$ be a conformal triangulation of Ω into triangles K.
- We consider piecewise finite elements and we denote u_h the obtained solution.
- We introduce anisotropic error estimates the involved constants being independent of the aspect ratio, provided the "mesh is aligned with the solution".
- We use the anisotropic interpolation error of Formaggia and Perotto (2001,2003).

Error estimator: linear $-\nabla \cdot (\mu \nabla u) = f$

- Let $f \in L^2(\Omega)$, $\mu \in W^{1,\infty}(\Omega)$, $u \in H_0^1(\Omega)$ solution of the problem and u_h the finite element solution.
- Assume that there exists $\hat{C} > 0$ depending only on the reference triangle $\hat{K}$ such that for any $K \in \mathcal{T}_h$ we have $\lambda_{1,K}^2 \mathbf{r}_{1,K}^T G_K(u-u_h)\mathbf{r}_{1,K} \leq \hat{C}\lambda_{2,K}^2 \mathbf{r}_{2,K}^T G_K(u-u_h)\mathbf{r}_{2,K}$.



$$(G_K(u-u_h))_{ij} = \int_{\Delta K} \frac{\partial(u-u_h)}{\partial x_i}\frac{\partial(u-u_h)}{\partial x_j}.$$

- Then there exists $\hat{C}_1$, $\hat{C}_2$ independent of the mesh size and aspect ratio such that up to higher order terms (Dubuis, Passelli, Picasso 2022)

$$\hat{C}_1 \int_\Omega \mu|\nabla(u-u_h)|^2 \leq \sum_{K\in\mathcal{T}_h} \eta_K^2 \leq \hat{C}_2 \int_\Omega \mu|\nabla(u-u_h)|^2,$$

$$\eta_K^2 = \Big(||\Pi_K f + \Pi_K \nabla\mu \cdot \nabla u_h||_{L^2(K)} + \frac{1}{2}\sum_{i=1}^{3}\left(\frac{|l_i|}{\lambda_{1,K}\lambda_{2,K}}\right)^{1/2} ||[\Pi_{l_i}\mu\nabla u_h \cdot \mathbf{n}]||_{L^2(l_i)}\Big) \sum_{i=1}^{2} \lambda_{i,K}^2 \mathbf{r}_{i,K}^T G_k(u-u_h)\mathbf{r}_{i,K}$$

Adaptive strategy

- Goal: construct a mesh such that

$$0.75\text{TOL} \leq \left(\frac{\sum_{K \in \mathcal{T}_h} \eta_K^2}{\int_\Omega \mu |\nabla u_h|^2} \right)^{1/2} \leq 1.25\text{TOL}$$

- Strategy: iteratively solve the problem and change the mesh:
  - Equidistribute the error in both directions for each triangle
  - Align directions $\mathbf{r}_{1,K}$ and $\mathbf{r}_{2,K}$ with respect to eigenvectors of $G_k(u - u_h)$

Numerical results

Consider $\Omega = (0,1)^2$ with f such that u is

$$u(\mathbf{x}) = \mu_2 \sin(\pi x_1) H_\varepsilon(x_1 - 0.5) + \mu_1 \sin(\pi x_1) H_\varepsilon(0.5 - x_1),$$

$$\mu(\mathbf{x}) = \mu_2 H_\varepsilon(x_1 - 0.5) + \mu_1 (1 - H_\varepsilon(x_1 - 0.5))$$

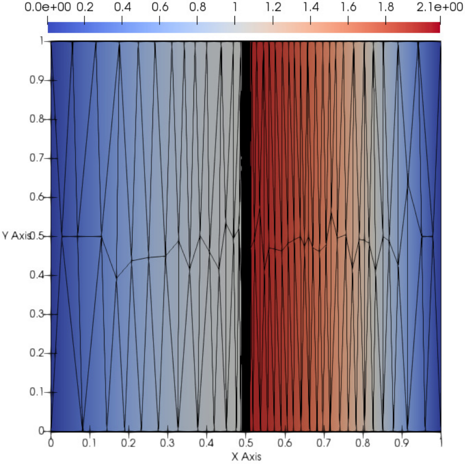
where for all $x \in \mathbb{R}$ and $\varepsilon > 0$ we define a smoothing of the classical Heavyside function.

$$H_\epsilon(x) = \begin{cases} 0 & x \leq -\epsilon, \\ \frac{x+\epsilon}{2\epsilon} + \frac{1}{2\pi}\sin\left(\frac{\pi x}{\epsilon}\right) & -\epsilon \leq x \leq \epsilon, \\ 1 & \epsilon \leq x. \end{cases}$$

$\mu_1 = 1$ $\mu_2 = 2$ $\epsilon = 0.01$ Starting mesh 10×10 uniform

TOL	Vertices	ei^A	e_{H^1}	ei^{ZZ}	$\mathrm{ar}_{\max}$	$\mathrm{ar}_{\mathrm{av}}$
0.0125	741	0.96	0.054	1.00	17847	3055
0.00625	1388	0.99	0.027	1.00	37973	6683
0.003125	2822	0.98	0.013	1.00	77257	13292
$\mu_1 = 1$ $\mu_2 = 100$ $\epsilon = 0.01$ Starting mesh 10×10 uniform						
0.0125	524	1.02	7.34	0.98	17609	4046
0.00625	1070	1.03	3.82	0.98	35918	7553
0.003125	2166	1.03	1.86	0.99	91030	15305

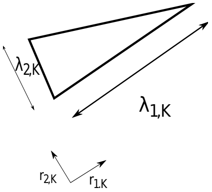
Adapted mesh



- Obtained adapted mesh at tolerance $\mathrm{TOL} = 0.025$.

Error estimator: $-\nabla \cdot ((\mu_0 + |\nabla u|^{p-2})\nabla u) = f$

- $f \in L^q(\Omega)$ $(\frac{1}{p} + \frac{1}{q} = 1)$, let $u \in W_0^{1,p}(\Omega)$ be a solution of the problem and u_h the finite element solution of the finite variational problem.
- We can prove the following upper bound



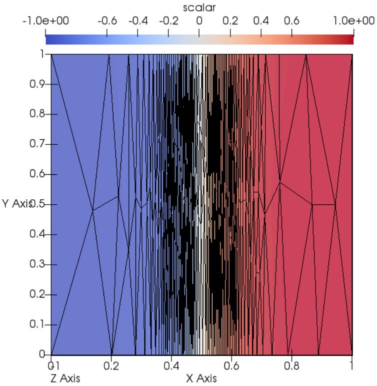
$$\int_\Omega |\nabla(u-u_h)|^2(\mu_0 + |\nabla u| + |\nabla(u-u_h)|) \le \hat{C} \sum_{K \in \mathcal{T}_h} \eta_K \tag{1}$$

$$\eta_K = \Big(||\nabla \cdot ((\mu_0 + |\nabla u_h|)\nabla u_h) + f||_{L^2(K)} + \frac{1}{2\lambda_{2,K}^{1/2}} ||[(\mu_0 + |\nabla u_h|)\nabla u_h \cdot \mathbf{n}]||_{L^2(\partial K)} \Big) \sum_{i=1}^{2} \lambda_{i,K}^2 \mathbf{r}_{i,K}^T G_k(u-u_h)\mathbf{r}_{i,K}.$$

- $(G_K(u-u_h))_{ij} = \int_{\Delta K} \frac{\partial(u-u_h)}{\partial x_i} \frac{\partial(u-u_h)}{\partial x_j}$.
- $\int_\Omega |\nabla(u-u_h)|^2(\mu_0 + |\nabla u| + |\nabla(u-u_h)|)$ is a quasi-norm (Liu, Yan, 2001).

Numerical results

TOL	ei^A	e_{QN}	ei^{ZZ}
$\mu_0 = 0$			
0.125	13.32	0.78	0.88
0.0625	18.68	0.20	1.00
0.03125	18.55	0.08	1.00
0.015625	17.02	0.04	0.99
$\mu_0 = 1$			
0.125	16.62	0.31	1.00
0.0625	18.68	0.25	0.99
0.03125	15.60	0.11	1.00
0.015625	19.09	0.052	0.97
$\mu_0 = 100$			
0.125	10.97	5.63	0.98
0.0625	10.90	2.55	0.98
0.03125	11.03	1.23	0.99
0.015625	9.91	0.65	0.97



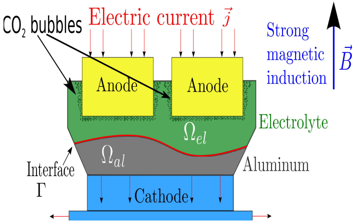
- Obtained adapted mesh at tolerance TOL$= 0.125$ $\mu_0 = 0$

- Exact solution: $u(x, y) = \tanh\left(\frac{x-0.5}{0.1}\right)$.

Application to aluminium electrolysis

EPFL

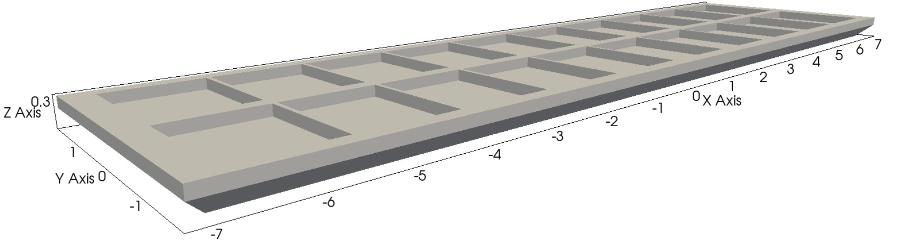
- Consider $\Omega = \Omega_{\mathrm{al}} \cup \Omega_{\mathrm{el}}$.
- A free interface problem should be considered, here the interface Γ is considered flat and fixed.
- $\epsilon_{ij}(\mathbf{u}) = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})\ i, j = 1, 2, 3.$



$$
\begin{aligned}
\rho(\mathbf{u}\cdot\nabla)\mathbf{u} - \nabla\cdot(2\mu\epsilon(|u|)\epsilon(u)) + \nabla p = \rho\mathbf{g} + \mathbf{j}\wedge\mathbf{B} \qquad & \text{in } \Omega, \\
\nabla\cdot\mathbf{u} = 0 \qquad & \text{in } \Omega.
\end{aligned}
$$

- Two models are considered
  - Smagorinsky $\mu(|\epsilon(\mathbf{u})|) = \mu_L + C|\epsilon(\mathbf{u})|$ (Application of the modified p-Laplace problem presented before).
  - Von Karmann $\mu(|\epsilon(\mathbf{u})|) = \mu_L + Cd^2_{\partial\Omega}|\epsilon(\mathbf{u})|$ (ongoing work).

Application to aluminium electrolysis



Comparison between adapted mesh and standard one

- Results obtained on the standard mesh and adapted mesh show similar accuracy.
- An adapted mesh could be used for several simulations.

Mesh	N. vertices	Adaptation CPU time	CPU time updating interface
Standard	326099	-	6h11
Adapted	41687	3h33m	1h12

Adapted mesh vs standard mesh

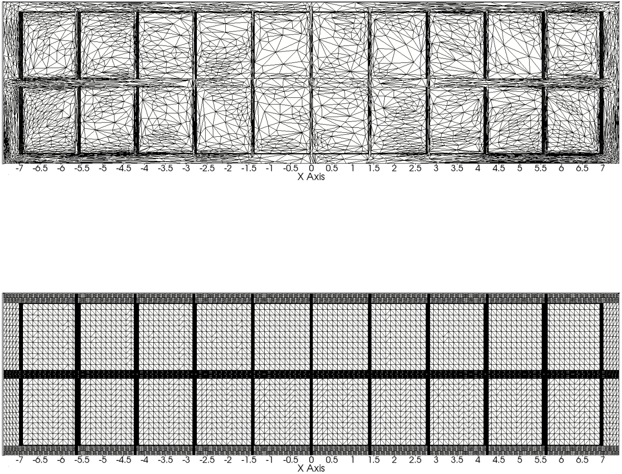


Figure: Top: Adapted mesh Bottom: Standard mesh. View from above.

Adapted mesh vs standard mesh

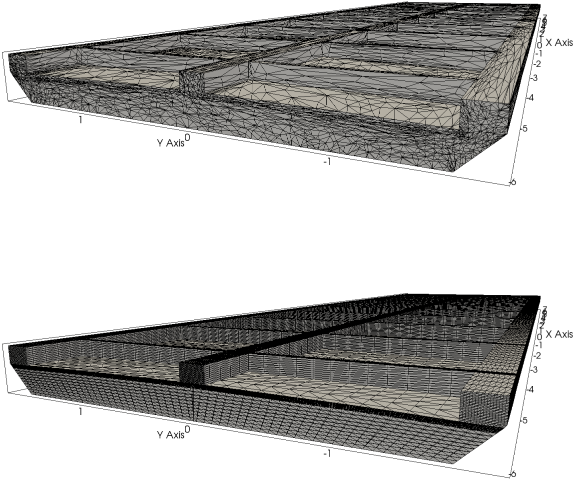


Figure: Top: Adapted mesh Bottom: Standard mesh.

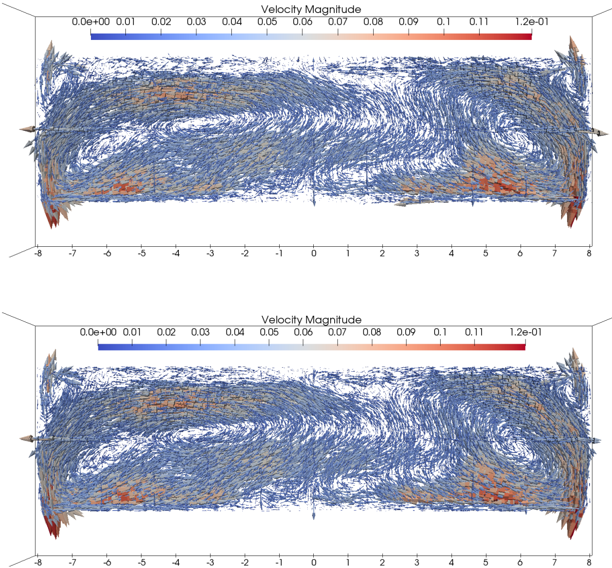


Figure: Top: Adapted mesh Bottom: Standard mesh. View from above.

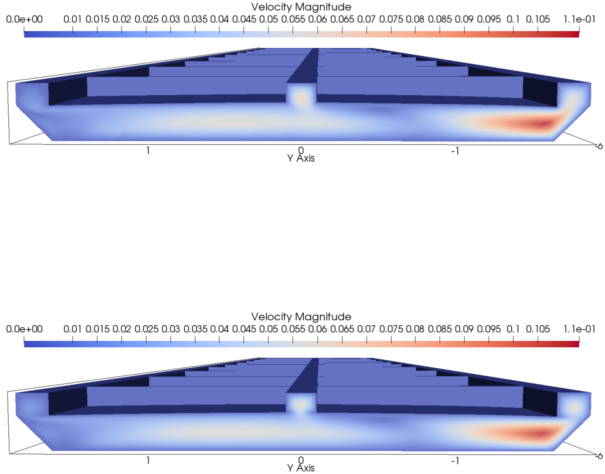


Figure: Top: Adapted mesh Bottom: Standard mesh.

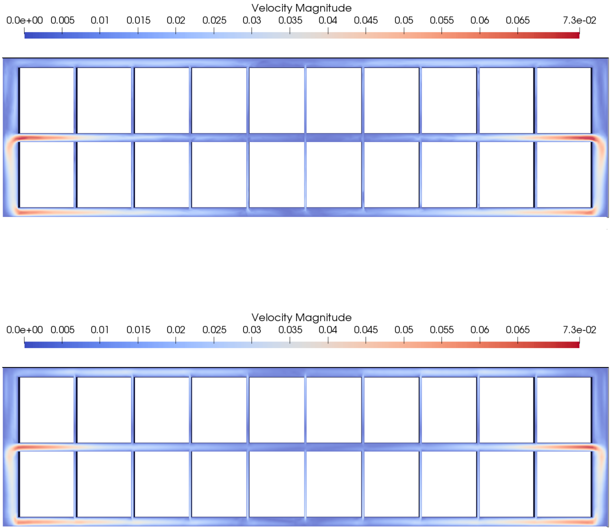


Figure: Top: Adapted mesh Bottom: Standard mesh. Cut view from below.

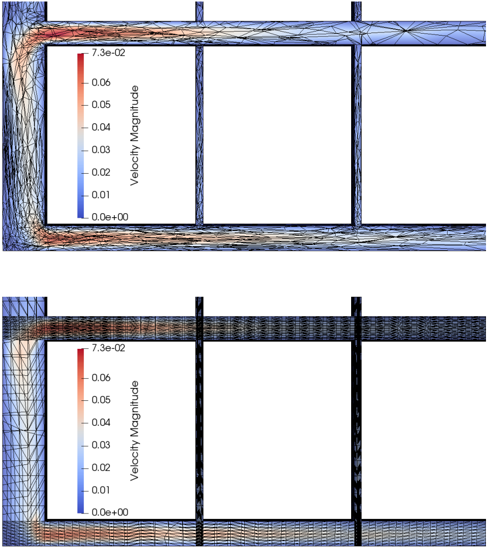


Figure: Top: Adapted mesh Bottom: Standard mesh. Zoom cut view from below.

Conclusion and further work

- With the help of adaptive finite elements with large aspect ratio the accuracy can be controlled reducing considerably the CPU time.
- The effectivity index does not depends on the aspect ratio on adapted meshes.
- The efficiency of the algorithm has been validated on an industrial application.
- We are working on the theoretical framework of the Von Karmann model, where the distance of the wall is involved in the turbulence model.

Thank you!