International Conference on Adaptive Modeling and Simulation
ADMOS 2021
F. Larsson and P. Díez

ADAPTIVE FINITE ELEMENTS WITH LARGE ASPECT RATIO FOR ALUMINIUM ELECTROLYSIS

PARIDE PASSELLI* AND MARCO PICASSO†

* Institute of Mathematics, EPFL, 1015 Lausanne, Switzerland
e-mail: paride.passelli@epfl.ch, web page: http://people.epfl.ch/paride.passelli

† Institute of Mathematics, EPFL, 1015 Lausanne, Switzerland
e-mail: marco.picasso@epfl.ch, web page: http://people.epfl.ch/marco.picasso

Key words: A posteriori error estimates, Adaptive algorithm, Anisotropic finite elements, aluminium electrolysis

Abstract. An anisotropic adaptive algorithm to solve the Stokes problem is presented. The algorithm is based on an a posteriori error indicator justified in [10]. Numerical experiments in flat domains show that the error indicator is sharp. The adaptive algorithm is then used in the framework of aluminium electrolysis. Given the force field, a simplified Stokes problem is solved and an anisotropic adapted mesh is produced. The adapted mesh is then used to solve the industrial fluid-flow problem. Numerical experiments show that the CPU time is reduced while keeping the same accuracy than the standard non adapted mesh.

1 INTRODUCTION

Aluminium electrolysis is a multiphysics problem (heat and fluid flow, electromagnetism, chemistry) which involves multi-scale features (from meters to millimeters). The goal of this work is to construct anisotropic meshes for the fluid-flow problem arising from aluminium electrolysis. Given the force field, a simplified Stokes problem is solved and an anisotropic mesh is produced on the basis of an error indicator justified in [10]. The adapted mesh will then be used to solve the industrial fluid-flow problem. With this approach we aim to reduce the CPU time while controlling the precision of the solution. The outline will be the following: first we introduce the anisotropic adaptive algorithm for the simplified Stokes problem. Then we will present numerical results corresponding to aluminium electrolysis.

2 AN ANISOTROPIC ADAPTIVE ALGORITHM FOR THE STOKES PROBLEM

Consider $\Omega \subset \mathbb{R}^3$ a polyhedral domain. Let $\mu > 0$ and $\mathbf{f} : \Omega \to \mathbb{R}^3$, we search for $\mathbf{u} : \Omega \to \mathbb{R}^3$ and $p : \Omega \to \mathbb{R}$ such that

$$-\mu\Delta\mathbf{u} + \nabla p = \mathbf{f}, \quad \text{in } \Omega, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega, \tag{2}$$

$$\mathbf{u} = 0, \quad \text{on } \partial\Omega. \tag{3}$$

Let $V = (H_0^1(\Omega))^3$ and $Q = L_0^2(\Omega)$ the variational problem reads: look for $(\mathbf{u}, \mathbf{p}) \in V \times Q$ such that for all $(\mathbf{v}, q) \in V \times Q$ we have

$$a(\mathbf{u}, p; \mathbf{v}, q) = F(\mathbf{v}, q),$$

where

$$a(\mathbf{u}, p; \mathbf{v}, q) = \int_\Omega \big(\mu\nabla\mathbf{u}\nabla\mathbf{v} - p\nabla\cdot\mathbf{v} - (\nabla\cdot\mathbf{u})q\big)d\mathbf{x} \quad \text{and} \quad F(\mathbf{v}, q) = \int_\Omega \mathbf{f}\mathbf{v}d\mathbf{x}.$$

For any $0 < h < 1$ let $\mathcal{T}_h$ be a conforming mesh of $\bar{\Omega}$ into tetrahedra with diameter less than h. For any tetrahedron $K \in \mathcal{T}_h$ we define its size $\lambda_{i,K}$ in the stretching direction $\mathbf{r}_{i,K}$ with $i = 1, 2, 3$ as in [4, 5]. We consider continuous, piecewise linear stabilized finite elements and define the corresponding finite dimensional subspace $V_h \times Q_h \subset V \times Q$. We are therefore looking for $(\mathbf{u}_h, p_h) \in V_h \times Q_h$ such that for all $(\mathbf{v}_h, q_h) \in V_h \times Q_h$ we have

$$a_h(\mathbf{u}_h, p_h; \mathbf{v}_h, q_h) = F_h(\mathbf{v}_h, q_h),$$

where we define

$$\begin{aligned} a_h(\mathbf{u}_h, p_h; \mathbf{v}_h, q_h) &= a(\mathbf{u}_h, p_h; \mathbf{v}_h, q_h) \\ &\quad - \sum_{K\in\mathcal{T}_h} \alpha\frac{\lambda_{3,K}^2}{\mu}\int_K(-\mu\Delta\mathbf{u}_h + \nabla p_h)(-\mu\Delta\mathbf{v}_h + \nabla q_h)d\mathbf{x} \end{aligned}$$

and

$$F_h(\mathbf{v}_h, q_h) = F(\mathbf{v}_h, q_h) - \sum_{K\in\mathcal{T}_h} \alpha\frac{\lambda_{3,K}^2}{\mu}\int_K \mathbf{f}(-\mu\Delta\mathbf{v}_h + \nabla q_h)d\mathbf{x},$$

the parameter α being dimensionless and set once for all by the user. The problem is stable and convergent in the framework of anisotropic meshes, see [7]. We introduce now the anisotropic error indicator for the Stokes problem, for which an upper bound has been proved in [10]. The local error indicator η_K^2 is defined as

$$\eta_K^2 = \rho_K\omega_K(\mathbf{u} - \mathbf{u}_h), \tag{4}$$

where

$$\rho_K = ||\frac{1}{\mu}(\mathbf{f} - \nabla p_h) + \Delta \mathbf{u}_h||_{L^2(K)} + \frac{1}{2\sqrt{\lambda_{3,K}}}||[\nabla \mathbf{u}_h \cdot \mathbf{n}]||_{L^2(\partial K)},$$

$$\omega_K^2(\mathbf{v}) = \sum_{i,j=1}^{3} \lambda_{i,K}^2 (\mathbf{r}_{i,K}^T G_K(v_j) \mathbf{r}_{i,K}),$$

$$(G_K(v_j))_{k,l} = \int_{\Delta K} \frac{\partial v_j}{\partial x_k} \frac{\partial v_j}{\partial x_l} d\mathbf{x}, \quad k,l = 1,2,3.$$

Here $[\cdot]$ denotes the jump across an internal face and $\mathbf{n}$ is the unit edge normal. Estimator (4) still involves the continuous solution $\mathbf{u}$. Thus we still need to approximate the quantity $\omega_K(\mathbf{u} - \mathbf{u}_h)$. In practice we apply Zienkiewicz−Zhu (ZZ) post-processing techniques [14, 15, 16], which consist in replacing the first order partial derivatives of $(\mathbf{u} - \mathbf{u}_h)$ by their $L^2(\Omega)$ projection onto V_h, for details we refer to [8, 11, 9].

We briefly present an adaptive algorithm based on the above anisotropic error indicator. The MeshGems software [2] is used to generate anisotropic meshes, details can be found in [3]. The objective of the algorithm is to construct a mesh such that

$$0.75\mathrm{TOL} \leq \left(\frac{\sum_{K \in \mathcal{T}_h} \eta_K^2}{\int_\Omega \mu |\nabla \mathbf{u}_h|^2 d\mathbf{x}} \right)^{1/2} \leq 1.25\mathrm{TOL}. \tag{5}$$

For (5) to hold, we equidistribute the error in each tetrahedron $K \in \mathcal{T}_h$:

$$\frac{1}{N_h} 0.75^2 \mathrm{TOL}^2 \int_\Omega \mu |\nabla \mathbf{u}_h|^2 d\mathrm{x} \leq \eta_K^2 \leq \frac{1}{N_h} 1.25^2 \mathrm{TOL}^2 \int_\Omega \mu |\nabla \mathbf{u}_h|^2 d\mathbf{x},$$

where N_h is the number of tetrahedra in $\mathcal{T}_h$. As in [3] we equidistribute the error committed for each tetrahedron in each stretching direction $\mathbf{r}_{i,K}$, $i = 1,2,3$. In particular for each $K \in \mathcal{T}_h$ and $i = 1,2,3$ we require

$$\frac{1}{3N_h^2} 0.75^4 \mathrm{TOL}^4 \Big(\int_\Omega \mu |\nabla \mathbf{u}_h|^2 d\mathrm{x} \Big)^2 \leq \eta_{i,K}^4 \leq \frac{1}{3N_h^2} 1.25^4 \mathrm{TOL}^4 \Big(\int_\Omega \mu |\nabla \mathbf{u}_h|^2 d\mathbf{x} \Big)^2, \tag{6}$$

where we set

$$\eta_{i,K}^4 = \rho_K^2 \sum_{j=1}^{3} \lambda_{i,K}^2 (\mathbf{r}_{i,K}^T G_K(v_j) \mathbf{r}_{i,K}).$$

The strategy consists in (i) aligning each tetrahedron (its stretching directions) with the eigenvectors of G_K and (ii) based on (6) update the mesh size $\lambda_{i,K}$. This process is repeated until (5) is satisfied.

3 VALIDATION AND APPLICATION TO ALUMINIUM ELECTROLYSIS

3.1 Numerical study of the effectivity index for the Stokes problem on flat domain

We want to check the quality of our error indicator. Thus we define the so called effectivity index ei^{A},

$$\mathrm{ei}^{\mathrm{A}} = \frac{\left(\sum_{K \in \mathcal{T}_h} \eta_K^2\right)^{1/2}}{\left(\int_\Omega \mu |\nabla(\mathbf{u}-\mathbf{u}_h)|^2 d\mathbf{x}\right)^{1/2}}.$$

In order to verify the quality of the ZZ post processing, we define the ZZ effectivity index ei^{ZZ},

$$\mathrm{ei}^{ZZ} = \frac{\left(\int_\Omega |\nabla \mathbf{u}_h - \Pi_h^{ZZ} \nabla \mathbf{u}_h|^2\right)^{1/2}}{||\nabla(\mathbf{u}-\mathbf{u}_h)||_{L^2(\Omega)}},$$

where $\Pi_h^{ZZ}\nabla\mathbf{u}_h$ is the post processing of $\nabla\mathbf{u}_h$.

Consider problem (1)-(3) with a flat domain as in a Hall-Héroult cell: let $\Omega = (0,10)^2 \times (0,0.5)$, $\mu = 1$ and $\mathbf{f}$ be such that the exact solution of the problem is

$$\mathbf{u}_{\mathrm{ex}}(x,y,z) = \frac{1}{25^3}[4(y-10)^2 y(x-10)^2 x^2 (y-5), -4(x-5)y^2 x(y-10)^2(x-10), 0].$$

We choose a structured initial mesh of size $h_1, h_2, h_3 = 1, 1, 0.25$. The effectivity indices, the maximum and the average aspect ratio are reported in Table 1 when using several tolerances TOL (ar denotes the aspect ratio $\lambda_{1,K}/\lambda_{3,K}$). The ZZ error estimator is asymptotically exact (column four) and the error indicator presented does not dependent upon the mesh aspect ratio (column five). A cut at $x = 5$ of the mesh with computed solution at TOL$= 0.125$ is reported in Figure 1.

Table 1: Numerical results adaptive algorithm

TOL	# vertices	error H^1	ei^{ZZ}	ei^{A}	max ar	average ar
1.0	406	0.9.96	0.95	3.15	36.85	9.02
0.5	1838	4.09	0.96	3.01	67.69	9.23
0.25	7199	2.35	0.97	3.21	124.90	8.97
0.125	26524	1.18	0.98	3.25	183.79	9.50

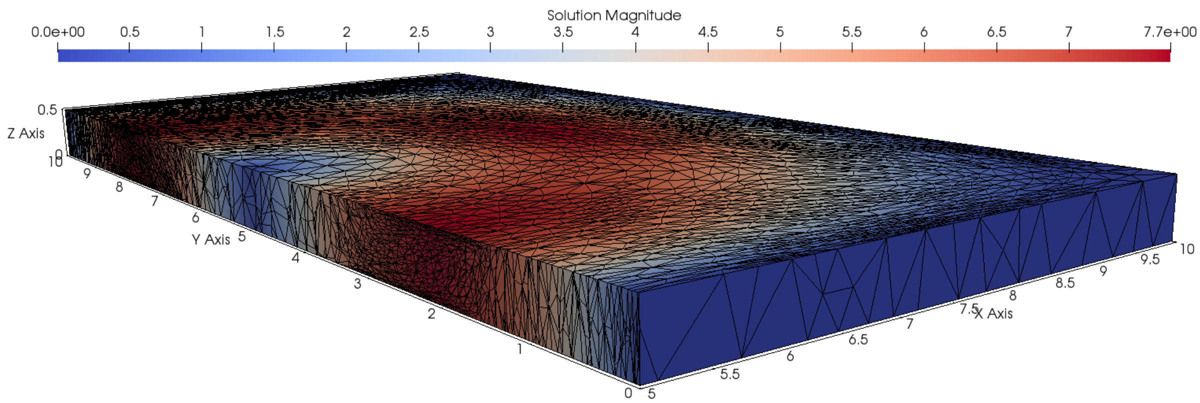

Figure 1: Cut of the adapted mesh when TOL= 0.125

3.2 Industrial application to an electrolysis cell

We now present numerical experiments of the industrial fluid-flow problem corresponding to aluminium electrolysis. The fluid domain is composed by two domains, one containing liquid aluminium and one containing liquid electrolyte (the so called bath). The velocity satisfies

$$\rho \cdot (\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot (2\mu\epsilon(\mathbf{u})) + \nabla p = \mathbf{F} \quad \text{in } \Omega, \tag{7}$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega, \tag{8}$$

where ρ the density and μ the viscosity, are piecewise constant in the bath and in the aluminium, and

$$\epsilon(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T).$$

The force term $\mathbf{F}$ acting on the fluids arises from gravity and Lorentz forces. A Smagorinski law is used to model turbulence. The model is implemented in the Alucell industrial software, see [13, 12, 6, 1] for details.

Given the force field $\mathbf{F}$, we solve the simplified Stokes problem (1)-(3) with $\mu = 1$ and adapt the mesh with the algorithm presented above. The obtained mesh when TOL= 0.5 is reported in Figure 2. The adapted mesh is then used to solve the fluid-flow problem (7)-(8). A cut of the standard non adapted mesh and the adapted mesh are shown in Figure 4. The standard mesh has approximately 320000 vertices, while the adapted mesh has only 31000 vertices. The CPU time needed to solve problem (7)-(8) with the standard mesh is about 13 hours, while it is only 2 hours for the adapted mesh. Both computations lead to a comparable velocity.

4 CONCLUSIONS

An anisotropic adaptive algorithm, based on a posteriori error indicator for the Stokes problem has been introduced. Numerical experiments on flat domains show the robustness

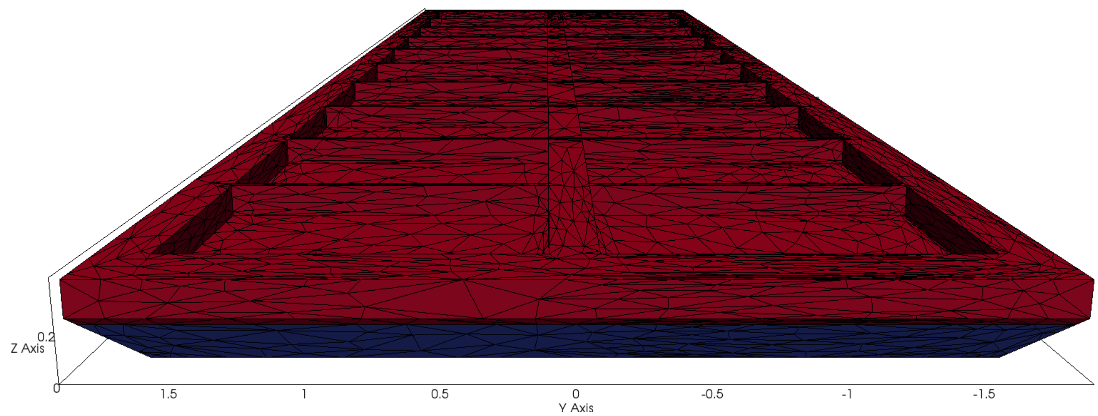

Figure 2: Adapted mesh when TOL=0.5

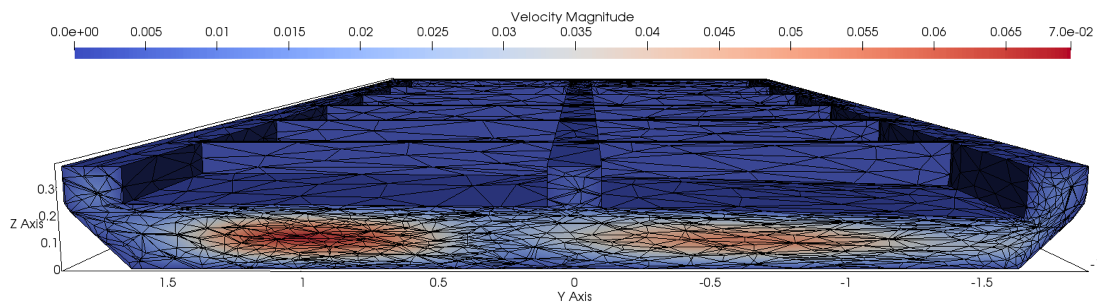

Figure 3: Cut at $x = -1$ of the adapted mesh when TOL=0.5

of the method. The method is then applied to aluminium electrolysis. The CPU time is reduced of a factor of 6.5 when using an adapted mesh while keeping the same accuracy.

We are studying the theoretical extension of this adaptive algorithm to the turbulent Navier-Stokes equations.

5 ACKNOWLEDGMENTS

Paride Passelli is financed by Rio Tinto Aluminium LRF Research Center at Saint Jean de Maurienne. The team of Rio Tinto Aluminium LRF in Saint-Jean de Maurienne is acknowledged for support. Jacques Rappaz is acknowledged for discussions.

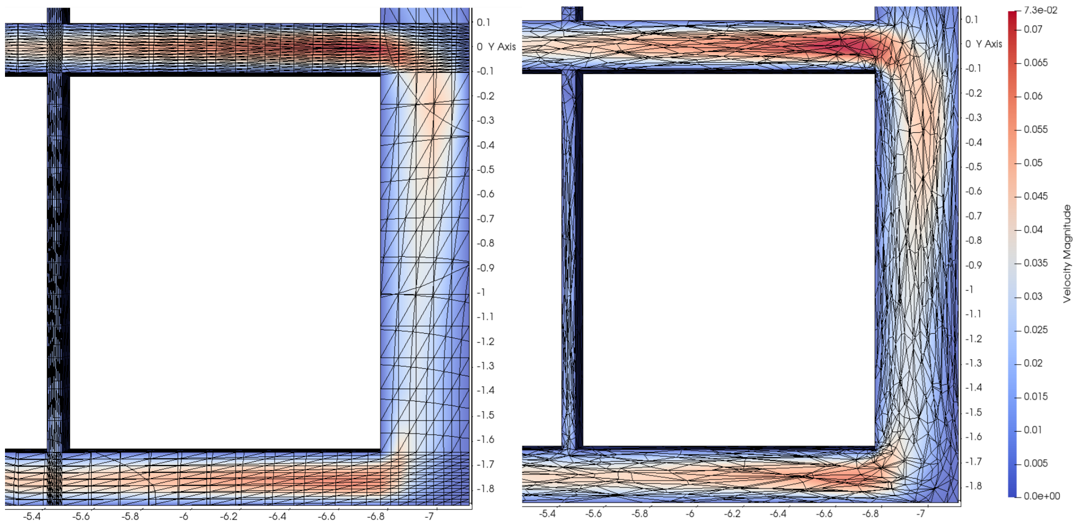

Figure 4: Cut at $z = 0.3$. Left: standard non adapted mesh. Right: adapted mesh when TOL= 0.5. Colors represent the velocity amplitude

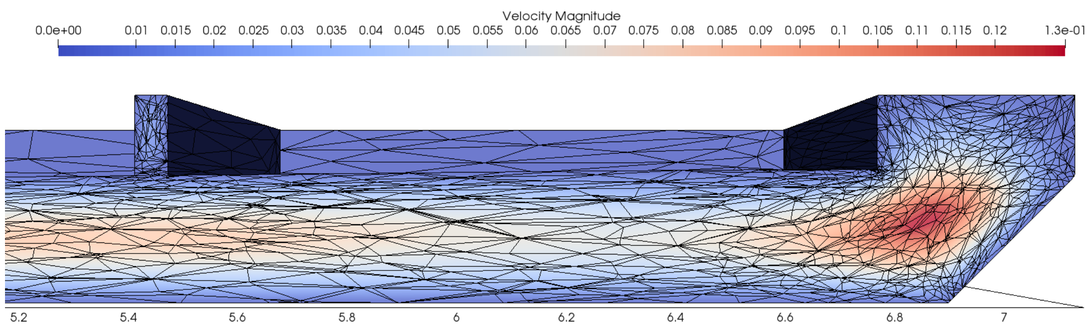

Figure 5: Cut at $y = -1$ of the adapted mesh when TOL=0.5

REFERENCES

[1] Descloux D., F.R.F.M.: A two fluids stationary free boundary problem. Comput. Methods Appl. Mech. Engrg. **77**, 215–226 (1989)

[2] Distene SAS: Meshgems suite 2.10. Release Notes (2019)

[3] Dubuis, S.: Adaptive algorithms for two fluids flows with anisotropic finite elements and order two time discretizations. Ph.D. thesis, Ecole polytechnique fédérale de Lausanne (2019)

[4] Formaggia, L., Perotto, S.: New anisotropic a priori error estimates. Numer. Math. **89**, 641–667 (2001)

[5] Formaggia, L., Perotto, S.: Anisotropic error estimates for elliptic problems. Numer. Math. **94**, 67–92 (2003)

[6] Gerbeau J.-F., B.C.L.T.: Mathematical methods for the magnetohydrodynamics of liquid metals. Math. Methods Magnetohydrodyn. Liquid Metals (2006)

[7] Micheletti, S., Perotto, S., Picasso, M.: Stabilized finite elements on anisotropic meshes : a priori error estimates for the advection-diffusion and the Stokes problems. SIAM J. Numer. Anal **41**(3), 1131–1162 (2003)

[8] Picasso, M.: Numerical study of the effectivity index for an anisotropic error indicator based on Zienkiewicz-Zhu error estimator. Commun. Numer. Meth. Engng **19**(1), 13–23 (2002)

[9] Picasso, M.: An anisotropic error estimator indicator based on Zienkiewicz-Zhu error estimator : application to elliptic and parabolic problems. SIAM J. Sci. Comput. **24**(4), 1328–1355 (2003)

[10] Picasso, M.: An adaptive algorithm for the Stokes problem unsing continuous, piecewise linear stabilized finite elements and meshes with high aspect ratio. Applied Numerical Mathematics **54**, 470–490 (2005)

[11] Picasso, M.: Adaptive finite elements with large aspect ratio based on an anisotropic error estimator involving first order derivatives. Comput. Methods Appl. Mech. Engrg. **196**, 14–23 (2006)

[12] Rochat, J.: Approximation numérique des écoulements turbulents dans des cuves d'électrolyse de l'aluminium. Ph.D. thesis, Ecole polytechnique fédérale de Lausanne (2016)

[13] Steiner, G.: Simulation numérique de phénomènes mhd: Application à l'électrolyse de l'aluminium. Ph.D. thesis, Ecole polytechnique fédérale de Lausanne (2009)

[14] Zienkiewicz, O.C., Zhu, J.Z.: A simple error estimator and adaptive procedure for practical engineering analysis. Int. J. Numer. Mehtods Engrg. **24**(2), 337–357 (1987)

[15] Zienkiewicz, O.C., Zhu, J.Z.: Analysis of the Zienkiewicz-Zhu a posteriori error estimator in the finite element method. Int. J. Numer. Mehtods Engrg. **28**(9), 2161–2174 (1989)

[16] Zienkiewicz, O.C., Zhu, J.Z.: The superconvergent patch recovery and a posteriori error estimates. I. the recovery technique. Int. J. Numer. Mehtods Engrg. **33**(7), 1331–1364 (1992)