

# Finite Volume Methods for the EMI Model of Electrophysiology : From Admissible to General Meshes

3<sup>rd</sup> MICROCARD Workshop / Strasbourg

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July 5, 2023

# Outline

- ▶ Model to be solved
- ▶ Finite Volume Schemes
- ▶ Convergence Analysis and Error Estimates
- ▶ Drawbacks of TPFA
- ▶ More Flexible Scheme
- ▶ Conclusion and Outlook

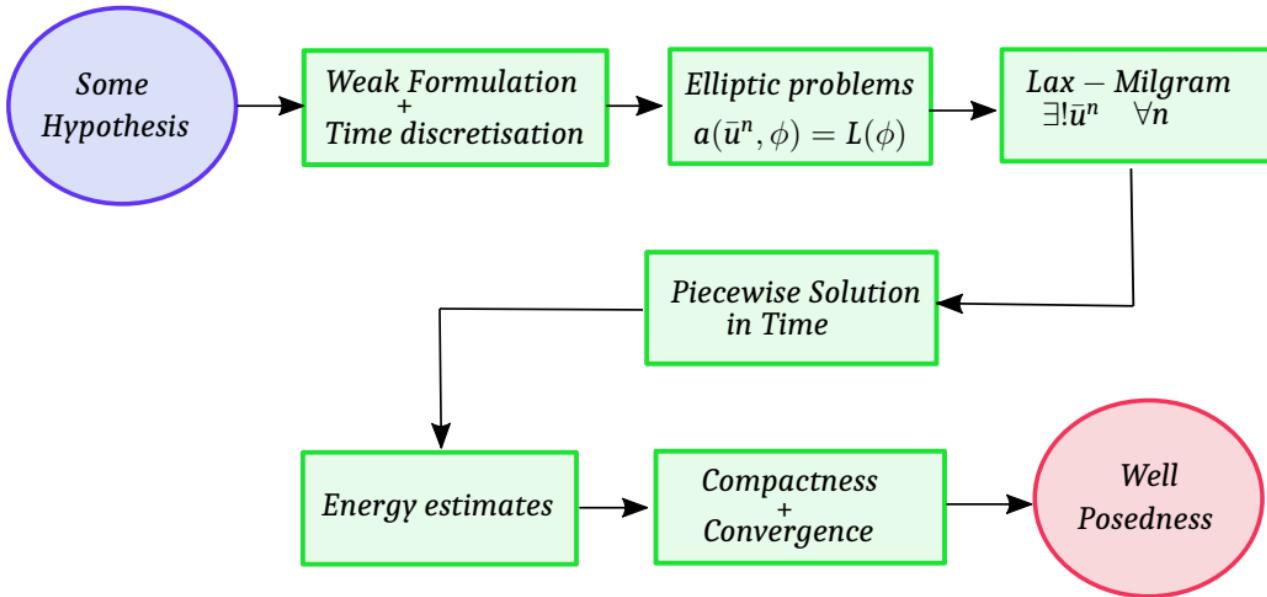
# Microscopic Bidomain Model

$$\begin{aligned}
 -\nabla \cdot (\sigma_k \nabla u_k) &= 0 && \text{in } \Omega_k, k = 0, 1, \\
 -\sigma_0 \nabla u_0 \cdot n_0 &= \sigma_1 \nabla u_1 \cdot n_1 = -(c_m \partial_t v + I_{\text{ion}}(v)) && \text{on } \Sigma := \overline{\Omega}_0 \cap \overline{\Omega}_1, \\
 -\sigma_0 \nabla u_0 \cdot n_0 &= g^N && \text{on } \Gamma_N \\
 u_0 &= g^D && \text{on } \Gamma_D \\
 v &= u_1 - u_0 && \text{on } \Sigma
 \end{aligned} \tag{1}$$



Figure: Geometrical set up of EMI model

# Well-Posedness of $\mu$ -Model<sup>1</sup>(One cell + Gap-junctions)



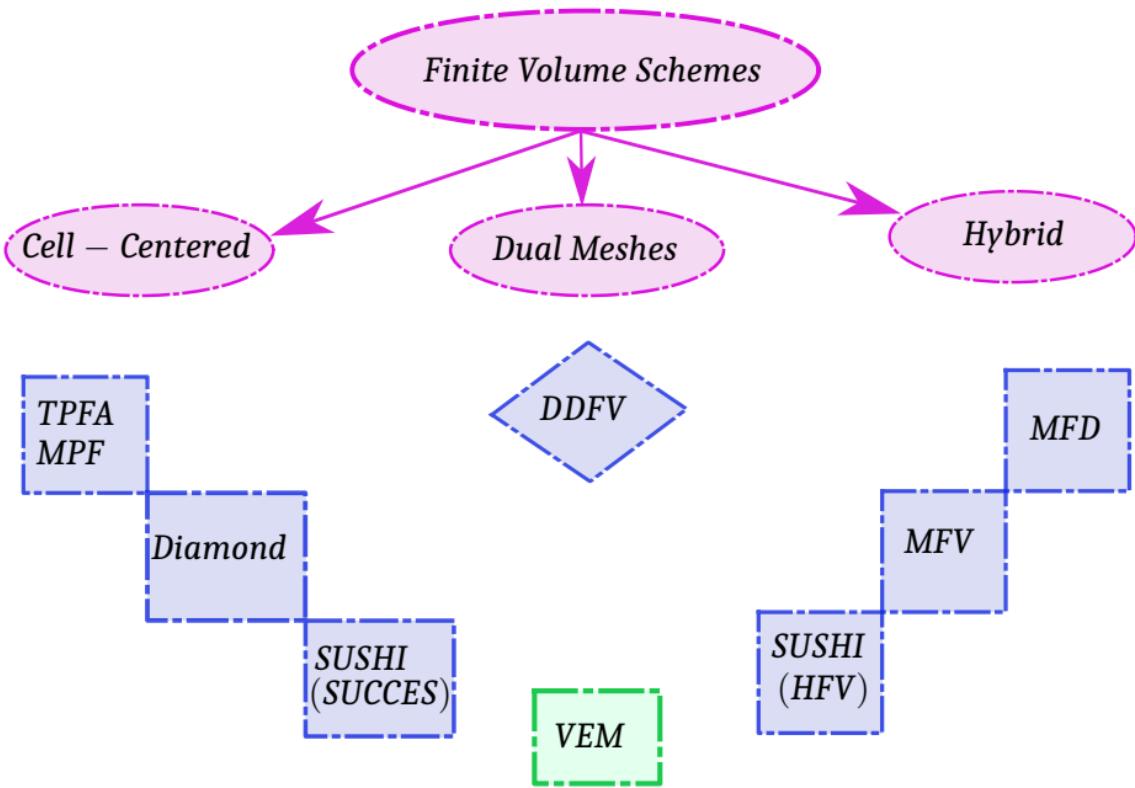
<sup>1</sup>P.E. Bécue. Modélisation et simulation de l'électrophysiologie cardiaque à l'échelle microscopique. UB, 2018.

# Finite Volume Methods

# Quick Bibliography

- ▶ Jerome Droniou, "Finite Volume Schemes for Diffusion Equations: Introduction to and Review of Modern Methods", 2014.
- ▶ Robert Eymard 1 , Thierry Gallouët 2 and Raphaële Herbin 3 October 2006. Finite Volume Methods. Handbook of Numerical Analysis, P.G. Ciarlet, J.L. Lions eds, vol 7, pp 713-1020.
- ▶ Jérôme Droniou, Robert Eymard, Thierry Gallouët, Cindy Guichard, Raphaele Herbin. The gradient discretisation method. Springer International Publishing AG, 82, 2018.

# Review Finite Volume



## Philosophy of the "Cell-Centered" FV Schemes

- ▶ Involve a single unknown  $u_K$  per  $K$ , taken as approximation of the value of  $u$  at each cell.
- ▶ Writing the balance equation over each cell, for which we associate the linear system.

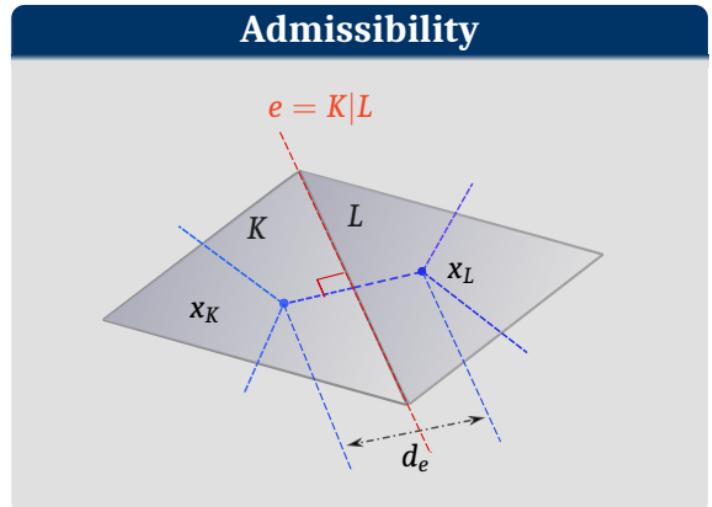
They are based on three principle ideas:

- ▶ Subdivision of the spatial domain into subsets called Control Volumes.
- ▶ Integration of the equation to be solved over the Control Volumes.
- ▶ Approximation of the derivative (flux) appearing after integration.

# Admissible<sup>2</sup> Orthogonal Meshes $(\mathcal{T}, \mathcal{E}, \mathcal{P})$

## Notations

- $\mathcal{T} = \mathcal{T}_0 \times \mathcal{T}_1 = \{K\}$ .
- $\mathcal{E} = \{e := K|L \text{ or } K|. \}$ .
- $\mathcal{P} = \{x_K \in K, \forall K \in \mathcal{T}\}$ .
- $\text{size}(\mathcal{T}) := \max_{K \in \mathcal{T}} \text{diam}(K)$ .
- $\mathcal{E} : \mathcal{E}_{\text{int}}^1, \mathcal{E}_{\text{int}}^0, \mathcal{E}_{\Sigma}, \mathcal{E}_{\text{ext}}^{\text{D}}, \mathcal{E}_{\text{ext}}^{\text{N}}$ .
- $|e|, |K|, n_{K,e}, d_e, d_{K,e}$ .
- $T = \Delta t N, t^n = n \Delta t, \forall n \in \{1, \dots, N\}$ .




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<sup>2</sup>R.Eymard, T. Gallouet and R. Herbin, Finite volume methods, October 2006. Handbook of Numerical Analysis, vol 7.

## Exact Balance Equations

The integral form of Eq (1.1) on "**any cell**  $K \in \mathcal{T}$ " at time  $t^n$  reads

$$-\sum_{e \in \mathcal{E}_K} \int_e \sigma_k \nabla u_k(t^n, \cdot) \cdot n_{Ke} = 0. \quad (2)$$

The integral of Eq (1.2) on "**any interface**  $e = K|L \in \mathcal{E}_\Sigma$ " at time  $t^n$  reads

$$-\int_e \sigma_0 \nabla u_0(t^n, \cdot) \cdot n_{Ke} = \int_e \sigma_1 \nabla u_1(t^n, \cdot) \cdot n_{Le} = - \left( c_m \int_e \partial_t v(t^n, \cdot) + \int_e I_{\text{ion}}(v(t^n, \cdot)) \right). \quad (3)$$

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$$-\bar{F}_{K,e}^n = \bar{F}_{L,e}^n = - \left( c_m \int_e \partial_t v(t^n, \cdot) + \int_e I_{\text{ion}}(v(t^n, \cdot)) \right). \quad (3)$$

# TPFA Finite Volume Scheme ( $N_{\mathcal{T}} \times N_{\Sigma}$ Eq)

## Discrete Balance Equations

We look for  $(u_{\mathcal{T}}^n, v_{\mathcal{T}}^n) \in \mathbb{R}^{\mathcal{T}} \times \mathbb{R}^{\Sigma}$ , such that  $\forall n \in \{1, \dots, N\}$

$$-\sum_{e \in \mathcal{E}_K} F_{Ke}^n = 0, \quad \text{for all } K \in \mathcal{T}, \quad (4)$$

$$-F_{Ke}^n = F_{Le}^n = -\left(\frac{c_m}{\Delta t}(v_e^n - v_e^{n-1}) + I_{\text{ion}}(v_e^{n-1})\right)|e|, \quad \text{for all } e = K|L \in \mathcal{E}_{\Sigma}, \quad (5)$$

Where the numerical flux  $F_{Ke}^n$  reads

$$F_{Ke}^n = \tau_e(u_L^n - u_K^n) \quad \text{if } e = K|L \in \mathcal{E}_K \cap \mathcal{E}^*, \quad K \in \mathcal{T}, \quad (6)$$

$$F_{Ke}^n = \tau_e(g_e^{D,n} - u_K^n) \quad \text{if } e = K| \in \mathcal{E}_K \cap \mathcal{E}_{\text{ext}}^D, \quad K \in \mathcal{T}_0, \quad (7)$$

$$F_{Ke}^n = -g_e^{N,n}|e| \quad \text{if } e = K| \in \mathcal{E}_K \cap \mathcal{E}_{\text{ext}}^N, \quad K \in \mathcal{T}_0, \quad (8)$$

$$F_{Ke}^n = \tau_e(u_L^n - u_K^n - v_e^n) \quad \text{if } e = K|L \in \mathcal{E}_K \cap \mathcal{E}_{\Sigma}, \quad K \in \mathcal{T}_0, \quad L \in \mathcal{T}_1 \quad (9)$$

The discrete balance equations (8)-(13) have a unique discrete solution  $(u_{\mathcal{T}}^n, v_{\mathcal{T}}^n)$ . (By R.E. & all)

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- ▶ Introduce the "auxiliary" unknowns  $u_{Ke}, u_{Le}$  s.t. :  $F_{Ke}^n = \tau_{Ke}(u_{K,e} - u_K^n), \quad F_{Le}^n = \tau_{Le}(u_{L,e} - u_L^n)$ .
- ▶ Thanks to  $F_{Ke}^n + F_{Le}^n = 0$ , one deduce  $\mathbf{u}_{K,e} = \frac{\tau_K}{\tau_K + \tau_L}u_K^n + \frac{\tau_L}{\tau_K + \tau_L}(u_L^n - v_e^n), \quad \mathbf{u}_{L,e} = \frac{\tau_K}{\tau_K + \tau_L}(u_K^n + v_e^n) + \frac{\tau_L}{\tau_L + \tau_L}u_L^n$

# Matrix Form

$$\begin{pmatrix} A & B \\ B^T & C + \frac{c_m}{\Delta t} |e| \text{Id}_{N_\Sigma} \end{pmatrix} \begin{pmatrix} u_{\mathcal{T}}^n \\ v_{\mathcal{T}}^n \end{pmatrix} = \begin{pmatrix} G^n \\ -\left(-\frac{c_m}{\Delta t} v_{\mathcal{T}}^{n-1} + I_{\text{ion}}(v_{\mathcal{T}}^{n-1})\right) |e| \end{pmatrix} \quad (10)$$

- ▶  $A$ : square matrix  $(N_{\mathcal{T}} \times N_{\mathcal{T}})$ , with  $a_{KL} = -\tau_e$  and  $a_{KK} = \sum_{e \in \mathcal{E}_K} \tau_e$ .
- ▶  $B$ : matrix  $(N_{\mathcal{T}} \times N_{\Sigma})$ , with  $b_{Ke} = \tau_e$  and  $b_{Le} = -\tau_e$ .
- ▶  $C$ : matrix  $(N_{\Sigma} \times N_{\Sigma})$ , with  $c_{ee} = \tau_e$ .
- ▶ Schur complement: matrix  $(N_{\Sigma} \times N_{\Sigma})$

$$\underbrace{(C - B^T A^{-1} B)}_{SC} v_{\mathcal{T}}^n = -|e| \frac{c_m}{\Delta t} (v_{\mathcal{T}}^n - v_{\mathcal{T}}^{n-1}) + |e| I_{\text{ion}}(v_{\mathcal{T}}^{n-1}) - B^T A^{-1} G^n.$$

Linear system (10) is SDP and coercive with a standard discrete  $H^1$  semi-norm and  $L^2$  norm.

# Convergence of TPFA Scheme

## Outline of the Proof ( $\mathbb{C}^2$ regularity)

- ▶ Defines errors associated with  $(u_{\mathcal{T}}^n, v_{\mathcal{T}}^n)$ .

$$\eta_{\mathcal{T}}^n = \bar{u}_{\mathcal{T}}^n - u_{\mathcal{T}}^n, \quad \epsilon_{\mathcal{T}}^n = \bar{v}_{\mathcal{T}}^n - v_{\mathcal{T}}^n.$$

# Convergence Analysis of TPFA Scheme

## Outline of the Proof ( $\mathbb{C}^2$ regularity)

- ▶ Defines errors associated with  $(u_{\mathcal{T}}^n, v_{\mathcal{T}}^n)$ .
- ▶ Compare  $\hat{F}_{K,e}^n$  with  $\bar{F}_{K,e}^n$ .

$$|e|R_{K,e}^n(u_0, u_1) = \hat{F}_{K,e}^n - \bar{F}_{K,e}^n.$$

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- ▶ Subtract the **discrete flux balance** equations from **exact flux balance**.

$$-\sum_{e \in \mathcal{E}_K} (\hat{F}_{Ke}^n - F_{Ke}^n) = -\sum_{e \in \mathcal{E}_K} |e| R_{Ke}^n,$$

$$-(\hat{F}_{Ke}^n - F_{Ke}^n) = -|e| R_{Ke}^n - (c_m T_e^n + S_e^n) |e| - \left( \frac{c_m}{\Delta t} (\eta_e^n - \eta_e^{n-1}) + I_{\text{ion}}(\bar{v}_e^{n-1}) - I_{\text{ion}}(v_e^{n-1}) \right) |e|.$$

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- ▶ Subtract the **discrete flux balance** equations from **exact flux balance**.
- ▶ Error estimate.

$$m' \Delta t |(\epsilon_{\mathcal{T}}^n, \eta_{\mathcal{T}}^n)|_{1,h}^2 + c_m \|\eta_{\mathcal{T}}^n\|_{0,\Sigma}^2 \leq c_m \left( 1 + \frac{\lambda}{c_m} \Delta t \right) \|\eta_{\mathcal{T}}^{n-1}\|_{0,\Sigma} \|\eta_{\mathcal{T}}^n\|_{0,\Sigma} + \Delta t R^n |(\epsilon_{\mathcal{T}}^n, \eta_{\mathcal{T}}^n)|_{1,h} \\ + \Delta t (c_m \|T_{\mathcal{T}}^n\|_{0,\Sigma} + \|S_{\mathcal{T}}^n\|_{0,\Sigma}) \|\eta_{\mathcal{T}}^n\|_{0,\Sigma},$$

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- ▶ Subtract the **discrete flux balance** equations from **exact flux balance**.
- ▶ Error estimate.
- ▶ Extracting two inequalities.

$$\|\eta_{\mathcal{T}}^n\|_{0,\Sigma} \leq \underbrace{\exp\left(\frac{3}{2}\frac{\lambda}{c_m}T\right)\left(\|\eta_{\mathcal{T}}^0\|_{0,\Sigma}^2 + \frac{1}{m'c_m}R_{\mathcal{T}}^2 + \frac{2c_m}{\lambda}T_{\mathcal{T}}^2 + \frac{2}{\lambda c_m}S_{\mathcal{T}}^2\right)^{1/2}}_{\theta(\text{size}(\mathcal{T})+\Delta t)} \quad (11)$$

$$\Delta t \sum_{n=1}^N |(\eta_{\mathcal{T}}^n, \epsilon_{\mathcal{T}}^n)|_{1,h}^2 \leq \underbrace{\frac{c_m}{m'}\|\eta_{\mathcal{T}}^0\|_{0,\Sigma}^2 + 2c_m^2 T_{\mathcal{T}}^2 + 2S_{\mathcal{T}}^2 + 2(\lambda+1)T \max_{n=1\dots N} \|\eta_{\mathcal{T}}^n\|_{0,\Sigma}^2}_{\theta(\text{size}(\mathcal{T})+\Delta t)} \quad (12)$$

# Convergence Analysis of TPFA Scheme

## Outline of the Proof ( $H^2$ regularity)

- ▶ Convex-hull for any  $K$ ,  
 $\mathcal{V}_{K,e} = \{sx + (1 - s)x_K, x \in e, s \in [0, 1]\}.$
- ▶ We assume without loss of generality the following geometry  $\Rightarrow$  Figure.
- ▶ Regularity conditions on the mesh + Technical computations.
- ▶ Consistency error  
 $|R_{K,e}^n| \leq C \frac{\text{size}\mathcal{T}}{(m(e)d_e)^{1/2}} \|u\|_{H^2(\mathcal{V}_{K,e})}.$
- ▶ Same generic form of the error estimates like above.

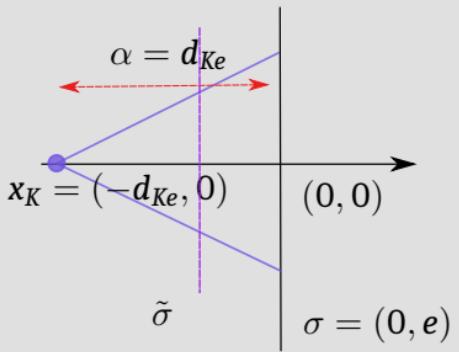


Figure: Convex-Hull

# Drawbacks of TPFA

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## How to find an admissible mesh

- ▶ Cartesian meshes: **OK ✓**.
- ▶ Non Cartesian quadrangle meshes:  
**IMPOSSIBLE**.
- ▶ Conforming triangular meshes: **OK ✓**,  
**BUT** (maybe  $d_e = 0$ ).
- ▶ Non Conforming triangular meshes :  
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## The discrete gradient is not good

- ▶ One direction of gradient approximation.
- ▶ Weak convergence of the gradient.

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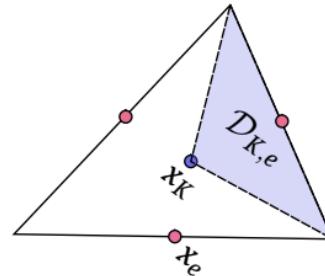
- ▶ One direction of gradient approximation.
- ▶ Weak convergence of the gradient.

⇒ **Approximation of the gradient using more than 2 points !!**

# Flexible scheme: SUSHI

## Toy Problem

$$\begin{aligned} -\operatorname{div}(\lambda(x) \nabla u) &= f, \text{ on } \Omega \\ u &= 0, \text{ on } \partial\Omega \end{aligned} \quad (13)$$



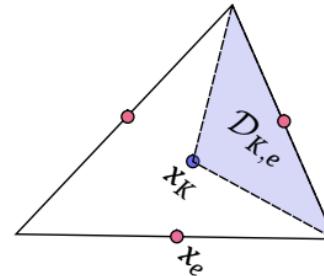

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<sup>3</sup>Discretisation of heterogeneous and anisotropic diffusion prb on general nonconforming meshes SUSHI R. E. & all.

# SUSHI<sup>3</sup> (Scheme Using Stabilization and Hybrid Interfaces)

## Toy Problem

$$\begin{aligned} -\operatorname{div}(\lambda(x) \nabla u) &= f, \text{ on } \Omega \\ u &= 0, \text{ on } \partial\Omega \end{aligned} \quad (13)$$



## Philosophy of SUSHI Scheme

- ▶ Weak formulation with discrete space  $\chi_{\mathcal{D},0} = \{(u_K, u_e) \in \mathbb{R}^{\mathcal{T}} \times \mathbb{R}^{\mathcal{E}}, u_e = 0, \forall e \in \mathcal{E}_{ext}\}$ .
- ▶ Unknowns on cells (**SUCCES**) and on interfaces (**HFV**).
- ▶ Set of edges splits on barycentric and hybrid edges  $\mathcal{E} = \mathcal{E}_B \cup \mathcal{E}_H; u_e = \sum_K \gamma_K^e u_K, \forall e \in \mathcal{E}_B$ .
- ▶ Geometric formula  $\Rightarrow \nabla_K u = \frac{1}{|K|} \sum_{e \in \mathcal{E}_K} |e| (u_e - u_K) n_{K,e}$ .

$\Rightarrow$  adapted to  $\mu$ -Model ?!

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## ► Conclusion

- Well-posedness of  $\mu$ -Model.
- TPFA Scheme on Admissible mesh
- Convergence Analysis via Error Estimates with different regularities.
- Extension to more flexible scheme with general meshes "SUSHI".

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## ► Ongoing

- Coding TPFA scheme (2D with triangular mesh, and 3D with FV5-point scheme with rectangular mesh).
- Working on the SUSHI scheme.
- Time integration IMEX or Rush-Larsen.

## ► Outlook

- Diamond Scheme.
- Implementation on OpenCarp?

- ▶ Conference Paper (**FVCA10 / Strasbourg**):
  - [Zeina CHEHADE](#) & Yves Coudière, "Two-Point Finite Volume Scheme for a Microscopic Bidomain Model of Electrophysiology".
- ▶ Article:
  - P.E. Béguin, [Zeina CHEHADE](#), Yves Coudière, "Existence of a Solution for a Microscopic Bidomain Model of Electrophysiology". ([Reduction](#))

# Thank You For Your Attention!



## Acknowledgment

This work was supported by the European High-Performance Computing Joint Undertaking EuroHPC under grant agreement No 955495 (MICROCARD) co-funded by the Horizon 2020 programme of the European Union (EU), the French National Research Agency ANR, the German Federal Ministry of Education and Research, the Italian ministry of economic development, the Swiss State Secretariat for Education, Research and Innovation, the Austrian Research Promotion Agency FFG, and the Research Council of Norway.



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