Convergence of finite volume schemes for the macroscopic bidomain model of the heart electric activity.

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and Computing in Electrocardiology
Plan of the talk

1. Model & Main Result
2. Mathematical setting revisited
3. Discrete Duality Finite Volume Schemes
   - Generalities on FV schemes
   - DDFV schemes: Pro&Contra
   - 2D DDFV
   - 3D DDFV
   - Discrete Calculus Tools
4. DDFV Scheme for the Model Problem
5. Convergence Analysis
   - The time-implicit case
   - The linearized implicit case
MODEL AND MAIN RESULTS
Problem considered...

We provide a convergence analysis of certain Finite Volume schemes (namely, different variants of DDFV schemes) for the problem \((\text{Prob})\):

\[
\partial_t v - \text{div} \, M_i(x) \nabla u_i + h(v) = l_{\text{app}}, \quad (t, x) \in Q_T,
\]

\[
- \partial_t v - \text{div} \, M_e(x) \nabla u_e - h(v) = -l_{\text{app}}, \quad (t, x) \in Q_T,
\]

with Neumann boundary conditions

\[
(M_i, e(x) \nabla u_{i,e}) \cdot n = s_{i,e} \quad \text{on} \ (0, T) \times \partial \Omega,
\]

and with initial datum: \(v(0, x) = v_0(x), \ x \in \Omega.\) Here:
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\[ \partial_t v - \text{div} \mathbf{M}_i(x) \nabla u_i + h(v) = I_{\text{app}}, \quad (t, x) \in Q_T, \]
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\[ (\mathbf{M}_{i,e}(x) \nabla u_{i,e}) \cdot n = s_{i,e} \quad \text{on} \quad (0, T) \times \partial \Omega, \]

and with initial datum: \( v(0, x) = v_0(x), \ x \in \Omega. \) Here:

- \( \Omega \) is a time-independent Lipschitz domain in \( \mathbb{R}^3 \) (the heart does not move...); the space-time domain is \( Q_T = (0, T) \times \Omega; \)
- \( u_i, u_e \) is the intra- (respectively, extra-) cellular electric potential;
- \( v := u_i - u_e \) is the transmembrane potential;
- \( I_{\text{app}}(t, x) \) is a given stimulation current;
- \( \mathbf{M}_i(x) \) and \( \mathbf{M}_e(x) \) are the intra- and extra-cellular conductivity tensors (assumed symmetric, positive definite, but anisotropic).
- \( h(v) \) is an *ad hoc* model for the transmembrane ionic current.

We focus on the case where \( h \) is close to a cubic polynomial.
Assumptions on the ionic current

We assume that \( h : \mathbb{R} \rightarrow \mathbb{R} \) is a continuous function, and there exist \( r \in (2, +\infty) \) and constants \( C, L, l > 0 \) such that

\[
\frac{1}{C} |v|^r \leq |h(v)v| \leq C (|v|^r + 1), \tag{1}
\]

\( \tilde{h} : z \mapsto h(z) + Lz + l \) is strictly increasing on \( \mathbb{R} \), with \( \tilde{h}(0) = 0 \). \( \tag{2} \)

In the known models, the appropriate value is \( r = 4 \); this means, the nonlinearity \( h \) is of cubic growth at infinity. Assumptions (1),(2) are automatically satisfied by any cubic polynomial \( h \) with positive leading coefficient.
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Our results will cover the cases

— of a general $r$, for the convergence of the fully implicit scheme;

— of $r < 4$ (strictly!), for the linearized implicit scheme.

There is some hope for attaining the critical case $r = 4$ (V.V. Zhikov’s lemmas...).
Main results

- We construct a simpler variant of the 3D Discrete Duality Finite Volume Scheme (very close to the scheme of Charles Pierre) and apply it to discretize \((Prob)\).
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- either as \([ h(\nu) ]_{n+1} = h(\nu^n) \) (time-explicit);
- or as \([ h(\nu) ]_{n+1} = h(\nu^{n+1}) \) (time-implicit);
- or as \([ h(\nu) ]_{n+1} = \frac{h(\nu^n) + Lv^n + I}{\nu^n} \nu^{n+1} - Lv^{n+1} - I \) (linearized implicit).
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  The scheme is time-implicit for the diffusion terms, and for the ionic current term we have (roughly speaking... we’ll focus on the details in the sequel of the talk) three choices:
  - either as \([ h(v) ]^{n+1} = h(v^n) \) (time-explicit);
  - or as \([ h(v) ]^{n+1} = h(v^{n+1}) \) (time-implicit);
  - or as \([ h(v) ]^{n+1} = \frac{h(v^n) + L v^n + l}{v^n} v^{n+1} - L v^{n+1} - l \) (linearized implicit).

- We have existence for each of the schemes.
- For the fully implicit scheme, we show convergence. Drawback: the scheme is nonlinear!
- For the linearized implicit scheme, we show convergence if \( r < 4 \) (whereas \( r = 4 \) is regarded as the practical case).

NB: In practice, the explicit discretization of the ionic current works (cf. Ch. Pierre), but we fail to prove a priori estimates.
MATHEMATICAL SETTING
Consider $V := H^1(\Omega)$ and the quotient space $V_0 := H^1 / \{ v \equiv \text{const} \}$. We denote by $V' := H^{-1}$ the dual space of $V$. 
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**Definition**

A weak solution to (Prob) is a triple of functions $(u_i, u_e, v) : \Omega \rightarrow \mathbb{R}^3$ such that $u_i, e \in L^2(0, T; V)$, $v = u_i - u_e$, $v \in L^r(Q)$, and (Prob) is satisfied in $\mathcal{D}'([0, T) \times \Omega)$. 
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We normalize $u_i$ by requiring that $\int_{\Omega} u_i(t, \cdot) = 0$ for a.e. $t \in (0, T)$. 
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It is convenient to give a “variational” formulation of (Prob).

The following spaces are (almost) relevant for the analysis of (Prob):

$$L^2(0, T; V) \cap L'(Q) \text{ and its dual space } L^2(0, T; V') + L^{r'}(Q);$$

the notation $< \cdot, \cdot >$ refers to their duality pairing.
Variational (re)formulation.

Remark

*If* \((u_i, u_e, v)\) *is a weak solution of* \((\text{Prob})\), *the system and initial condition are satisfied in the space* \(L^2(0, T; V') + L^r(Q)\), *i.e.* the distributional derivative \(\partial_t v\) *can be identified with an element of* \(L^2(0, T; V') + L^r(Q)\).
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**Remark**

If $(u_i, u_e, v)$ is a weak solution of (Prob), the system and initial condition are satisfied in the space $L^2(0, T; V') + L'^r(Q)$, i.e. the distributional derivative $\partial_t v$ can be identified with an element of $L^2(0, T; V') + L'^r(Q)$.

**With this identification,** one has for all $\varphi \in L^2(0, T; V) \cap L'^r(Q)$

$$
\int_0^T < \partial_t v, \varphi > + \iint_Q \left( M_i(x, \nabla u_i) \cdot \nabla \varphi + h(v) \varphi \right) - \int_0^T \int_{\partial \Omega} s_i \varphi = \iiint_Q l_{\text{app}} \varphi,
$$

$$
\int_0^T < \partial_t v, \varphi > - \iint_Q \left( M_e(x, \nabla u_e) \cdot \nabla \varphi + h(v) \varphi \right) + \int_0^T \int_{\partial \Omega} s_e \varphi = \iiint_Q l_{\text{app}} \varphi;
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\]

and for all \(\varphi \in L^2(0, T; V)\) such that \(\partial_t \varphi \in L^\infty(Q)\) and \(\varphi(T, \cdot) = 0\),

\[
\int_0^T \langle \partial_t v, \varphi \rangle = -\iint_Q v \partial_t \varphi - \int_\Omega v_0(\cdot) \varphi(0, \cdot).
\]
A regularization lemma. Well-posedness.

The following tool helps to work with the variational formulation.

**Lemma**

Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain. There exists a family of linear operators $(\mathcal{R}_\varepsilon)_\varepsilon$ acting from $L^2(0, T; V)$ into $\mathcal{D}(\mathbb{R} \times \mathbb{R}^d)$ such that
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- for all $w \in L^2(0, T; V)$, $\mathcal{R}_\varepsilon(w)$ converges to $w$ in $L^2(0, T; V)$;
- for all $w \in L^r(Q_T) \cap L^2(0, T; V)$, $\mathcal{R}_\varepsilon(w)$ converges to $w$ in $L^r(Q_T)$. 
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This lemma is used in order to regularize $u_{i,e}$, so that one could take $\mathcal{R}_\varepsilon(u_{i,e})$ as test functions in the equations $(Prob)$. E.g., a priori estimates on the weak solution are obtained in this way. Another application is the uniqueness theorem below.

**Theorem**

There exists at most one weak solution $(u_i, u_e, v)$ to $(Prob)$. 
A regularization lemma. Well-posedness.

Proof.

Take \( \zeta \in \mathcal{D}([0, T]) \). We take \( \zeta(t) \mathcal{R}_\varepsilon(u_i - \hat{u}_i)(t, x) \) as the test function in the first equation, and \( \zeta(t) \mathcal{R}_\varepsilon(u_e - \hat{u}_e)(t, x) \), in the second equation of (Prob). We subtract the equations obtained and let \( \varepsilon \to 0 \). By the linearity of \( \mathcal{R}_\varepsilon(\cdot) \) and the convergences of \( \mathcal{R}_\varepsilon \), using the chain rule we get as \( \varepsilon \to 0 \),

\[
\iint_Q - \frac{(v - \hat{v})^2}{2} \partial_t \zeta - \int_\Omega \frac{(v_0 - \hat{v}_0)^2}{2} \zeta(0) + \iint_Q (h(v) - h(\hat{v})) (v - \hat{v}) \\
+ \sum_{j=i,e} \iint_Q \left( (M_j(x) \nabla u_j - M_j(x) \nabla \hat{u}_j) \right) \cdot (\nabla u_j - \nabla \hat{u}_j) \leq 0.
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$$+ \sum_{j=i,e} \int\int_Q ((M_j(x)\nabla u_j - M_j(x)\nabla \hat{u}_j) \cdot (\nabla u_j - \nabla \hat{u}_j)) \leq 0.$$

For a.e. $t > 0$, letting $\zeta$ converge to the characteristic function of $[0, t]$, thanks to the monotonicity assumption on $\tilde{h}$ we deduce

$$\int_\Omega (v - \hat{v})^2(t) \leq \int_\Omega (v_0 - \hat{v}_0)^2 + 2L \int_0^t \int_\Omega (v - \hat{v})^2.$$

By the Gronwall inequality, we deduce $v = \hat{v}$.
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By the Gronwall inequality, we deduce \( v = \hat{v} \).

Then also \( \hat{u}_i = u_i \) because of the monotonicity assumption on \( M_i(x) \) and the normalization condition on \( u_i \); finally, \( \hat{u}_e = u_e \).

\( \diamond \)
Rq: if one replaces $\partial_t v$ by the backward time differencing

$$\partial_t^{n+1} v : v(\cdot, \cdot) \mapsto \frac{1}{t^{n+1} - t^n} \left[ v(t^{n+1}, \cdot) - v(t^n, \cdot) \right]$$

then...
Time-implicit discretization: a minimization problem!

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then... at each time step, we have to solve the optimization pb.:

find $\min_{\nu \times \nu} J^{n+1}$, where (given $\nu^n$)

$$J^{n+1}(u_i, u_e) := \int_\Omega \frac{1}{2} (u_i - u_e)^2 - \int_\Omega \nu^n(u_i - u_e)$$

$$+ (t^{n+1} - t^n) \int_\Omega \left( \frac{1}{2} \| M_i^{1/2} \nabla u_i \|^2 + \frac{1}{2} \| M_e^{1/2} \nabla u_e \|^2 + H(u_i - u_e) \right);$$

here $H$ is a primitive of $h$, $H : z \mapsto \int_0^z h(s) \, ds$. 
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then... at each time step, we have to solve the optimization pb.:

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$$+(t^{n+1} - t^n) \int_\Omega \left( \frac{1}{2} \| M_1^{1/2} \nabla u_i \|^2 + \frac{1}{2} \| M_e^{1/2} \nabla u_e \|^2 + H(u_i - u_e) \right);$$

here $H$ is a primitive of $h$, $H : z \mapsto \int_0^z h(s) \, ds$.

This feature will be preserved in our fully implicit scheme; thus the scheme (although non linear) can be solved by descent methods, since it derives from minimization of a coercive functional (NB: for time steps $(t^{n+1} - t^n)$ small enough, the functional $J^{n+1}$ will be strictly convex).
DDFV Schemes
We use Finite Volumes (FV, for short) for space discretization of (\textit{Prob}) for the time discretization, we’ll pick the (essentially implicit) Euler scheme. Thus we describe the scheme at one time step.

Generally, let us think of discretizing an elliptic equation of the kind

$$\quad u - \text{div } \mathcal{F} = f(x, u), \quad \mathcal{F} = A(x, u, \nabla u).$$
Generalities on FV schemes

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$$ u - \text{div} \mathcal{F} = f(x, u), \quad \mathcal{F} = A(x, u, \nabla u). $$

The principles for FV approximation of such equations are the following:

- A partition of the space domain $\Omega$ into “volumes” $\kappa$ is given; the partition is called “mesh” and denoted by $\mathcal{T}$.

- An unknown $u_\kappa$ is associated to each volume (usually regarded as the value at a “center” point of the volume, denoted $x_\kappa$); the whole set of the unknowns is called “discrete solution” and denoted by $u^\mathcal{T}$.
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- If \(\kappa, \lambda\) are “neighbours” (adjacent volumes), the divided differences \(\frac{u_\lambda - u_\kappa}{d_{\kappa\lambda}}\) are used to “reconstruct” the “discrete gradient” \(\nabla^\mathfrak{T}u^\mathfrak{T}\) of \(u^\mathfrak{T}\).
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NB: In the schemes we think of, the reconstruction is done “by hands”. We do not solve any equations to compute the values of \( \nabla^\mathcal{T} u^\mathcal{T} \) from those of \( u^\mathcal{T} \), but fix ad hoc formulas for \( \nabla^\mathcal{T} u^\mathcal{T} \) in terms of \( u^\mathcal{T} \).
Generalities on FV schemes

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- An unknown \( u_\kappa \) is associated to each volume (usually regarded as the value at a “center” point of the volume, denoted \( x_\kappa \)); the whole set of the unknowns is called “discrete solution” and denoted by \( u^{\mathcal{T}} \).
- If \( \kappa, L \) are “neighbours” (adjacent volumes), the divided differences \( \frac{u_L - u_\kappa}{d_{KL}} \) are used to “reconstruct” the “discrete gradient” \( \nabla^{\mathcal{T}} u^{\mathcal{T}} \) of \( u^{\mathcal{T}} \).

NB: In the schemes we think of, the reconstruction is done “by hands”. We do not solve any equations to compute the values of \( \nabla^{\mathcal{T}} u^{\mathcal{T}} \) from those of \( u^{\mathcal{T}} \), but fix \textit{ad hoc} formulas for \( \nabla^{\mathcal{T}} u^{\mathcal{T}} \) in terms of \( u^{\mathcal{T}} \).

Here we may have too much liberty! “DDFV” schemes we’ll use is one way to reconstruct, among many others.
Each couple of neighbour volumes possesses a part of the common border, called “interface” and denoted by $K_L$. Combining the values $u_K, u_L$ and the values of the reconstructed discrete gradient $\nabla^\Sigma u^\Sigma$ near $K_L$, we produce a discretization $F_{KL}$ of the flux $F = A(x, u, \nabla u)$ on $K_L$. 
Each couple of neighbour volumes possesses a part of the common border, called “interface” and denoted by $K_L$. Combining the values $u_K$, $u_L$ and the values of the reconstructed discrete gradient $\nabla^\Sigma u^\Sigma$ near $K_L$, we produce a discretization $\mathcal{F}_{K_L}$ of the flux $\mathcal{F} = A(x, u, \nabla u)$ on $K_L$.

In two steps, the PDE is replaced by a set of algebraic equations:

- Firstly, the PDE is “projected on the mesh”. One integrates the continuous equation on $\kappa$; the Green-Gauss formula is used to reduce $\int_K \text{div} \mathcal{F}$ to $\int_{\partial K} \mathcal{F} \cdot n$.
  
  This yields a discrete system of equalities, one per volume.

- And secondly, these equalities are approximated by replacing $u|_K$ with the unknown $u_K$ and replacing $\mathcal{F}|_{K_L}$ with the expression of $\mathcal{F}_{K_L}$ (in our setting, $\mathcal{F}_{K_L}$ is a closed-form formula involving $u_K$ and the neighbour unknowns $u_L$).

As a result, we obtain a closed system of algebraic equations which (hopefully...) can be solved, often in an approximate way. This yields $u^\Sigma$ (and also $\nabla u^\Sigma$) that may be viewed as approximations of $u$ and $\nabla u$, respectively...
Generalities on FV schemes (cont’d)

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Generalities on FV schemes (cont'd)

- Each couple of neighbour volumes possesses a part of the common border, called "interface" and denoted by $\kappa|\lambda$. Combining the values $u_\kappa$, $u_\lambda$ and the values of the reconstructed discrete gradient $\nabla^\Sigma u^\Sigma$ near $\kappa|\lambda$, we produce a discretization $\mathcal{F}_{\kappa|\lambda}$ of the flux $\mathcal{F} = A(x, u, \nabla u)$ on $\kappa|\lambda$.

- In two steps, the PDE is replaced by a set of algebraic equations:
  
  Firstly, the PDE is "projected on the mesh". One integrates the continuous equation on $\kappa$; the Green-Gauss formula is used to reduce $\int_\kappa \text{div} \mathcal{F}$ to $\int_{\partial \kappa} \mathcal{F} \cdot n$.

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  And secondly, these equalities are approximated by replacing $u|_\kappa$ with the unknown $u_\kappa$ and replacing $\mathcal{F}|_{\kappa|\lambda}$ with the expression of $\vec{\mathcal{F}}_{\kappa|\lambda}$ (in our setting, $\vec{\mathcal{F}}_{\kappa|\lambda}$ is a closed-form formula involving $u_\kappa$ and the neighbour unknowns $u_\lambda$).

- As a result, we obtain a closed system of algebraic equations which (hopefully...) can be solved, often in an approximate way. This yields $u^\Sigma$ (and also $\nabla u^\Sigma$) that may be viewed as approximations of $u$ and $\nabla u$, respectively... provided the "convergence" of the method can be justified.

We do not discuss the efficiency of different approximations, but only look at mathematical properties of the schemes that allow to justify the convergence.
Yet, let us point out some advantages and drawbacks for the schemes we’ll discuss compared to other schemes (other finite volume schemes, mimetic finite difference schemes, finite elements...)
Yet, let us point out some **advantages** and **drawbacks** for the schemes we’ll discuss compared to other schemes (other finite volume schemes, mimetic finite difference schemes, finite elements...)

- The scheme has many unknowns, more precisely, the interaction between the unknowns does not seem optimal
- Unless the mesh is “orthogonal” and the problem is isotropic, the **discrete maximum principle** for linear elliptic problems fails
- Many objects are introduced, and the notation is relatively heavy
- ...?
Yet, let us point out some **advantages** and **drawbacks** for the schemes we’ll discuss compared to other schemes (other finite volume schemes, mimetic finite difference schemes, finite elements...)

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- Many objects are introduced, and the notation is relatively heavy
- ...?

+ in FV, local conservativity is built in explicitly (which does not mean that, e.g., finite elements schemes are not locally conservative)

+ in the DDFV schemes, we have a naturally consistent discretization of the gradient, and in many cases, the discrete gradient converges strongly to the exact solution gradient
**DDFV : pro&contra (cont)**

+ **DDFV schemes support quite unstructured meshes** (non-orthogonal, non-conforming, locally refined)
+ **they work on heterogeneous, anisotropic linear problems** (like our (Prob) !) and on nonlinear problems (e.g., non-Newtonian fluids)
+ **numerical convergence rates on linear anisotropic diffusion problems are quite good** (up to $h^2$ order, cf. F. Hermeline)
DDFV: pro\&contra (contd)

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- convenient discrete calculus tools for DDFV schemes were developed.

Indeed, “DDFV” means “discrete duality finite volumes”, that is, a discrete analogue of the integration-by-parts formula is available.

The consequences are:
DDFV schemes: Pro & Contra (cont'd)

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Indeed, “DDFV” means “discrete duality finite volumes”, that is, a discrete analogue of the integration-by-parts formula is available. The consequences are:

- the key mathematical features that underlie the existence theory for (Prob) are preserved: coercivity, monotonicity, variational structure. This ensures that the scheme is unconditionally stable.
- The variational structure being preserved, the scheme (although not necessarily linear) derives from a convex minimization problem; therefore, the scheme can be efficiently solved.
- Calculations can be written in a concise and easy-to-interprete way, thanks to the far-reaching analogy between the continuous and the discrete frameworks.
The DDFV schemes were devised in 2D, first by F. Hermeline ’98, then rediscovered and popularized by K. Domelevo & P. Omnès ’05. Their introduction is due to the difficulties of approximation of the normal flux $\mathbf{F} \cdot n.$
The DDFV schemes were devised in 2D, first by F. Hermeline ’98, then rediscovered and popularized by K. Domelevo & P. Omnès ’05.

Their introduction is due to the difficulties of approximation of the normal flux \( \mathcal{F} \cdot n \):

- even for the laplacian (i.e., for \( \mathcal{F} = \nabla u \)), if the mesh is not “orthogonal”
- for anisotropic and/or heterogeneous linear pbs (\( \mathcal{F} = A(x) \nabla u \))
- for nonlinear problems (e.g., when \( \mathcal{F} = | \nabla u |^{p-2} \nabla u \))

in all these cases, the divided differences \( \frac{u_L - u_K}{d_{KL}} \) are not sufficient to approximate \( \mathcal{F} \cdot n \) on \( \mathcal{K} \).
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in all these cases, the divided differences \( \frac{u_K - u_L}{d_{KL}} \) are not sufficient to approximate \( \mathcal{F} \cdot n \) on \( K_L \).

Different FV schemes solving this difficulty were proposed by Coudière & Vila & Villedieu, Afif & Amaziane, Handlovicova & Mikula & Sgallari, Aavatsmark et al., A. & Gutnic & Wittbold, A. & Boyer & Hubert, Eymard & Droniou, Le Potier, ... and more recently, a number of schemes by Eymard & Gallouët & Herbin.
The idea of the “DDFV” schemes (which should rather be called “double” schemes) is to use the unknowns on both “primal” and “dual” meshes. This induces a partition of $\Omega$ into quadrilaterals called “diamonds” $D$; the discrete gradient is reconstructed diamond-wise, using the divided differences along the diagonals of $D$. 
In 2D, we reconstruct the discrete gradient on $D$ (and hence also on $K|L$ and $K|L^*$) from the two given projections:

\[
\nabla^\Xi u^\Xi |_{K|L} = \nabla^\Xi u^\Xi |_{K^*|L^*}
\]

\[
= \nabla^\Xi u^\Xi |_{D_{K^*|L^*}^{K|L}} = \text{the vector of } \mathbb{R}^2 \text{ with the projections } \begin{cases} 
\frac{u_L - u_K}{d_{KL}}, & \text{on } x_K \rightarrow x_L \\
\frac{u_{L^*} - u_{K^*}}{d_{K^*|L^*}}, & \text{on } x_{K^*} \rightarrow x_{L^*}.
\end{cases}
\]
DDFV in dimension two (cont\textsuperscript{d})

On the preceding figures, the \textbf{primal mesh} (denoted $\mathcal{M}$) consists of triangles, and the \textbf{dual mesh} (denoted $\mathcal{M}^*$) has the vertices of primal volumes $\kappa \in \mathcal{M}$ for centers $x_{\kappa^*}$ of dual volumes $\kappa^*$, and it has the primal centers $x_{\kappa}$ for vertices of the dual volumes $\kappa^*$.

Because the \textbf{discrete gradient} has been reconstructed on each primal interface $\kappa \mid \mathcal{L}$ and on each dual interface $\kappa^* \mid \mathcal{L}^*$, we can “integrate” the diffusion term $-\text{div} \ \mathcal{F} \equiv -\text{div} \ A(x, u, \nabla u)$ on each primal volume $\kappa$ and on each dual volume $\kappa^*$. This yields a closed system of equations on

$$u^\Xi := \left( (u_{\kappa})_{\kappa \in \mathcal{M}}, (u_{\kappa^*})_{\kappa^* \in \mathcal{M}^*} \right).$$
DDFV in 2D: discrete duality features

Notice that in the DDFV approach, the field $\mathcal{F}$ is discretized with one vector value per diamond $D \in \mathcal{D}$. In general, we will say that a vector-valued set $(\vec{F}_D)_{D \in \mathcal{D}}$ is a discrete function, denoted by $\vec{F}^\Xi$. 
Notice that in the DDFV approach, the field $\mathcal{F}$ is discretized with one vector value per diamond $D \in \mathcal{D}$. In general, we will say that a vector-valued set $(\vec{F}_D)_{D \in \mathcal{D}}$ is a discrete function, denoted by $\vec{F}$. 

The discrete gradient $\nabla^\mathcal{D}$ can be seen as an operator acting from the space $\mathbb{R}^\mathcal{D}$ of discrete functions to the space $(\mathbb{R}^2)^\mathcal{D}$ of discrete fields.

Reciprocally, the standard FV discrete divergence operator $\text{div}^\mathcal{D}$ acts from the space $(\mathbb{R}^2)^\mathcal{D}$ of discrete fields to the space $\mathbb{R}^\mathcal{D}$ of discrete functions.
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In order to state the discrete duality, we introduce two scalar products:

- for discrete functions $w^\mathcal{D}, v^\mathcal{D} \in \mathbb{R}^\mathcal{D}$,
  \[ [w^\mathcal{D}, v^\mathcal{D}] = \frac{1}{2} \sum_{K \in \mathcal{M}} m_K w_K v_K + \frac{1}{2} \sum_{K^* \in \mathcal{M}^*} m_{K^*} w_{K^*} v_{K^*}; \]

- for discrete fields $\vec{F}^\mathcal{D}, \vec{G}^\mathcal{D} \in (\mathbb{R}^2)\mathcal{D}$,
  \[ \{\vec{F}^\mathcal{D}, \vec{G}^\mathcal{D}\} = \sum_{D \in \mathcal{D}} m_D \vec{F}_D \cdot \vec{G}_D; \]
Notice that in the DDFV approach, the field $\mathcal{F}$ is discretized with one vector value per diamond $D \in \mathcal{D}$. In general, we will say that a vector-valued set $(\bar{\mathcal{F}}_D)_{D \in \mathcal{D}}$ is a discrete function, denoted by $\bar{\mathcal{F}}^\tau$. The discrete gradient $\nabla^\tau$ can be seen as an operator acting from the space $\mathbb{R}^\tau$ of discrete functions to the space $(\mathbb{R}^2)^\mathcal{D}$ of discrete fields.

Reciprocally, the standard FV discrete divergence operator $\text{div}^\tau$ acts from the space $(\mathbb{R}^2)^\mathcal{D}$ of discrete fields to the space $\mathbb{R}^\tau$ of discrete functions.

In order to state the discrete duality, we introduce two scalar products:

- for discrete functions $w^\tau, v^\tau \in \mathbb{R}^\tau$,
  \[
  \left[ [ w^\tau, v^\tau ] \right] = \frac{1}{2} \sum_{K \in \mathcal{M}} m_K \, w_K \, v_K + \frac{1}{2} \sum_{K^* \in \mathcal{M}^*} m_{K^*} \, w_{K^*} \, v_{K^*} ;
  \]

- for discrete fields $\bar{\mathcal{F}}^\tau, \bar{\mathcal{G}}^\tau \in (\mathbb{R}^2)^\mathcal{D}$,
  \[
  \left\{ \bar{\mathcal{F}}^\tau, \bar{\mathcal{G}}^\tau \right\} = \sum_{D \in \mathcal{D}} m_D \, \bar{\mathcal{F}}_D \cdot \bar{\mathcal{G}}_D ;
  \]

**Proposition (The Discrete Duality property)**

The discrete divergence and gradient operators $-\text{div}^\tau, \nabla^\tau$ are linked by

\[
\forall \, w^\tau \in \mathbb{R}_0^\tau \quad \forall \, \bar{\mathcal{F}}^\tau \in (\mathbb{R}^2)^\mathcal{D} \quad \left[ - \text{div}^\tau [ \bar{\mathcal{F}}^\tau ] , w^\tau \right] = \left\{ \bar{\mathcal{F}}^\tau , \nabla^\tau w^\tau \right\}.
\]
In 3D, the primal mesh $\mathcal{M}$ consists of tetrahedra; the description of the dual mesh $\mathcal{M}^*$ is a bit tedious. A generic dual volume $\kappa^*$ consists of all “elements” having $x_{\kappa^*}$ for a vertex; a generic element is depicted on the figure:
In 3D, the primal mesh $\mathcal{M}$ consists of tetrahedra; the description of the dual mesh $\mathcal{M}^*$ is a bit tedious. A generic dual volume $\kappa^*$ consists of all “elements” having $x_{\kappa^*}$ for a vertex; a generic element is depicted on the figure:

Similarly to the 2D case, a 3D diamond $D = D_{K^*,L^*,M^*}^{K,L}$

– isolates the interaction of neighbours $K, L$ and dual neighbours $K^*, L^*, M^*$;

– serves to reconstruct the discrete gradient $\nabla^\mathcal{M} u^\mathcal{M}$ of a discrete function $u^\mathcal{M}$.
3D DDFV

DDFV in dimension three

In 3D, the primal mesh $\mathcal{M}$ consists of tetrahedra; the description of the dual mesh $\mathcal{M}^*$ is a bit tedious. A generic dual volume $\kappa^*$ consists of all “elements” having $x_{\kappa^*}$ for a vertex; a generic element is depicted on the figure:

Similarly to the 2D case, a 3D diamond $D = D_{K^*,L^*,M^*}^{K,L}$
– isolates the interaction of neighbours $K, L$ and dual neighbours $K^*, L^*, M^*$;
– serves to reconstruct the discrete gradient $\nabla^\xi u^\xi$ of a discrete function $u^\xi$.

Similarly, a 3D subdiamond $s = s_{K^*,L^*}^{K,L}$
– isolates the interaction of neighbours $K, L$ and dual neighbours $K^*, L^*$;
– serves to reconstruct the discrete divergence $\text{div}^\xi \vec{F}^\xi$ of a discrete field $\vec{F}^\xi$. 
DDFV in dimension three (cont’d)

(a) 2D (sub)diamond.

(b) 3D primal volumes, diamond, subdiamond.
DDFV in dimension three (cont^d)

(c) 2D (sub)diamond.  
(d) 3D primal volumes, diamond, subdiamond.

Analogous gradient reconstruction applies in 3D, namely for $D = D_{K^*,L^*,M^*}^{K,L}$, 

$$\nabla^\times \vec{u}^\times |_D = \text{the vector of } \mathbb{R}^3 \text{ with the projections}$$

$$\left\{ \begin{array}{c} \frac{u_L - u_K}{d_{KL}}, \text{ on } \overrightarrow{x_K x_L} \\ \frac{u_{L^*} - u_{K^*}}{d_{K^*L^*}}, \text{ on } \overrightarrow{x_{K^*} x_{L^*}} \\ \frac{u_{K^*} - u_{M^*}}{d_{M^*K^*}}, \text{ on } \overrightarrow{x_{M^*} x_{K^*}} \\ \text{etc.} \end{array} \right.$$
In order to state the discrete duality and take into account the Neumann boundary condition, we need three scalar products:

- For 3D discrete functions $w^x, v^x \in \mathbb{R}^x$,
  \[
  \begin{bmatrix} w^x, v^x \end{bmatrix} = \frac{1}{3} \sum_{K \in \Omega} m_K \, w_K \, v_K + \frac{2}{3} \sum_{K^* \in \Omega^*} m_{K^*} \, w_{K^*} \, v_{K^*};
  \]

- For discrete fields $\vec{F}^x, \vec{G}^x \in (\mathbb{R}^3)^x$,
  \[
  \left\{ \vec{F}^x, \vec{G}^x \right\} = \sum_{D \in \mathcal{D}} m_D \, \vec{F}_D \cdot \vec{G}_D;
  \]
3D DDFV

**DDFV in 3D: discrete duality features**

In order to state the discrete duality and take into account the Neumann boundary condition, we need three scalar products:

- For 3D discrete functions \( w^\mathcal{T}, v^\mathcal{T} \in \mathbb{R}^\mathcal{T} \),
  \[
  \left[ w^\mathcal{T}, v^\mathcal{T} \right] = \frac{1}{3} \sum_{K \in \mathcal{M}} m_K \ w_K v_K + \frac{2}{3} \sum_{K^* \in \mathcal{M}^*} m_{K^*} \ w_{K^*} v_{K^*};
  \]
- For discrete fields \( \vec{F}^\mathcal{T}, \vec{G}^\mathcal{T} \in (\mathbb{R}^3)^\mathcal{T} \),
  \[\{ \vec{F}^\mathcal{T}, \vec{G}^\mathcal{T} \} = \sum_{D \in \mathcal{D}} m_D \ \vec{F}_D \cdot \vec{G}_D;\]
- For boundary Neumann datum \( s^\mathcal{T} \) and boundary trace \( w^{\partial \mathcal{T}} \) of \( w^\mathcal{T} \),
  \[\langle s^\mathcal{T}, w^{\partial \mathcal{T}} \rangle := \sum_{K \in \partial \mathcal{M}} s_K \ \int_K w^{\partial \mathcal{T}};\]
In order to state the discrete duality and take into account the Neumann boundary condition, we need three scalar products:

- for 3D discrete functions \( w^z, v^z \in \mathbb{R}^z \),
  \[
  \begin{bmatrix}
    w^z, v^z
  \end{bmatrix} = \frac{1}{3} \sum_{K \in \Omega} m_K w_K v_K + \frac{2}{3} \sum_{K^* \in \Omega^*} m_{K^*} w_{K^*} v_{K^*};
  \]

- for discrete fields \( \vec{F}^z, \vec{G}^z \in (\mathbb{R}^3)^z \),
  \[
  \{ \vec{F}^z, \vec{G}^z \} = \sum_{D \in \Delta} m_D \vec{F}_D \cdot \vec{G}_D;
  \]

- for boundary Neumann datum \( s^z \) and boundary trace \( w^{\partial z} \) of \( w^z \),
  \[
  \langle s^z, w^{\partial z} \rangle := \sum_{K \in \partial \Omega} s_K \int_K w^{\partial z},
  \]

Here the function \( w^z \) on \( \Omega \) appears naturally:

\[
  w^z = \frac{1}{3} \sum_{K \in \Omega} w_K 1_K + \frac{2}{3} \sum_{K^* \in \Omega^*} w_{K^*} 1_{K^*} = \frac{1}{3} w^{\Omega} + \frac{2}{3} w^{\Omega^*}
\]

and \( w^{\partial z} \) is its restriction on \( \partial \Omega \) (or, more precisely, its trace).
In order to state the discrete duality and take into account the Neumann boundary condition, we need three scalar products:

- for 3D discrete functions $w^x, v^x \in \mathbb{R}^x$, 
  \[ \left[ w^x, v^x \right] = \frac{1}{3} \sum_{K \in \mathcal{M}} m_K w_K v_K + \frac{2}{3} \sum_{K^* \in \mathcal{M}^*} m_{K^*} w_{K^*} v_{K^*}; \]

- for discrete fields $\vec{F}^x, \vec{G}^x \in (\mathbb{R}^3)^x$, 
  \[ \left\{ \vec{F}^x, \vec{G}^x \right\} = \sum_{D \in \mathcal{D}} m_D \vec{F}_D \cdot \vec{G}_D; \]

- for boundary Neumann datum $s^x$ and boundary trace $w_{\partial x}$ of $w^x$, 
  \[ \left\langle s^x, w_{\partial x} \right\rangle := \sum_{K \in \partial \mathcal{M}} s_K \int_K w_{\partial x}, \]

Here the function $w^x$ on $\Omega$ appears naturally:

\[ w^x = \frac{1}{3} \sum_{K \in \mathcal{M}} w_K 1_{l_K} + \frac{2}{3} \sum_{K^* \in \mathcal{M}^*} w_{K^*} 1_{l_{K^*}} = \frac{1}{3} w^{\mathcal{M}} + \frac{2}{3} w^{\mathcal{M}^*} \]

and $w_{\partial x}$ is its restriction on $\partial \Omega$ (or, more precisely, its trace).

**Proposition (The Discrete Duality property)**

*For all $w^x \in \mathbb{R}^x$ and all $\vec{F}^x \in (\mathbb{R}^3)^x$ such that $\vec{F}^x \cdot \vec{n}|_{\partial \Omega} = s^x$,*

\[ \left[ - \text{div}^x [\vec{F}^x], w^x \right] = \left\{ \vec{F}^x, \nabla^x w^x \right\} - \left\langle s^x, w_{\partial x} \right\rangle. \]
Along with the Discrete Duality, the following properties of the DDFV discretizations underlie the convergence proof. Consider a family $(\Xi_h)_{h \downarrow 0}$ of DDFV meshes with vanishing mesh size parameter $h$. 
Along with the Discrete Duality, the following properties of the DDFV discretizations underlie the convergence proof. Consider a family \((\mathcal{T}_h)_{h \downarrow 0}\) of DDFV meshes with vanishing mesh size parameter \(h\).

**Proposition (Consistency of the discrete gradient)**

Assume \(w \in L^p(\Omega), p < \infty\).

Denote \(w_K := \frac{1}{m_K} \int_{m_K} w, \quad w_{K^*} := \frac{1}{m_{K^*}^*} \int_{m_{K^*}^*} w\).

Set

\[ w^{m,h} := (w_K)_{K \in \mathcal{M}_h} \quad (\text{assimilated to } \sum_{K \in \mathcal{M}_h} w_K 1_{1_K}), \]

\[ w^{m^*,h} := (w_{K^*})_{K^* \in \mathcal{M}^*_h} \quad (\text{assimilated to } \sum_{K^* \in \mathcal{M}^*_h} w_{K^*} 1_{1_{K^*}}), \]

\[ w^{\mathcal{T},h} := (w^{m,h}, w^{m^*,h}) \quad (\text{assimilated to } \frac{1}{d} w^{m,h} + \frac{d-1}{d} w^{m^*,h}). \]
Discrete calculus tools

Along with the Discrete Duality, the following properties of the DDFV discretizations underlie the convergence proof. Consider a family \((\mathfrak{T}_h)_{h \downarrow 0}\) of DDFV meshes with vanishing mesh size parameter \(h\).

**Proposition (Consistency of the discrete gradient)**

Assume \(w \in L^p(\Omega), p < \infty\).

Denote
\[
  w_K := \frac{1}{m_K} \int_{m_K} w, \quad w_{K^*} := \frac{1}{m_{K^*}} \int_{m_{K^*}} w.
\]

Set
\[
  w^{m_h} := (w_K)_{K \in m_h} \quad \text{(assimilated to } \sum_{K \in m_h} w_K 1_{l_K}),
\]
\[
  w^{m^*_h} := (w_{K^*})_{K^* \in m^*_h} \quad \text{(assimilated to } \sum_{K^* \in m^*_h} w_{K^*} 1_{l_{K^*}}),
\]
\[
  w^{\mathfrak{T}_h} := (w^{m_h}, w^{m^*_h}) \quad \text{(assimilated to } \frac{1}{d} w^{m_h} + \frac{d-1}{d} w^{m^*_h}).
\]

- Then \(w^{m_h} \to w\) and \(w^{m^*_h} \to w\) in \(L^p(\Omega)\).
- Moreover, if \(\nabla w \in L^q(\Omega)\), then \(\nabla^{\mathfrak{T}_h} w^{\mathfrak{T}_h} \to \nabla w\) in \(L^q(\Omega)\), \(q < \infty\).
Proposition (Asymptotic $W^{1,p}$ compactness)

Assume $(w^\Xi_h)_{h \downarrow 0}$ is a sequence of discrete functions on DDFV meshes $\Xi_h$ such that

$$
\| \nabla^\Xi_h w^\Xi_h \|_{L^p(\Omega)} := \sum_{D \in \mathcal{D}_h} m_D |\nabla_D w^\Xi_h|^p \leq \text{const},
$$

and also $\| w^{\ominus_{\Omega}} h \|_{L^p(\Omega)}$, $\| w^{\ominus_{\Omega}^*} h \|_{L^p(\Omega)} \leq \text{const}$, where $p \in [1, \infty)$. 

Discrete calculus tools (cont'd)
Proposition (Asymptotic $W^{1,p}$ compactness)

Assume $(w^{\mathcal{X}_h})_{h} \downarrow 0$ is a sequence of discrete functions on DDFV meshes $\mathcal{X}_h$ such that

$$\| \nabla^{\mathcal{X}_h} w^{\mathcal{X}_h} \|_{L^p(\Omega)} := \sum_{D \in \mathcal{X}_h} m_D |\nabla_D w^{\mathcal{X}_h}|^p \leq \text{const},$$

and also $\| w^{m_h} \|_{L^p(\Omega)}, \| w^{m^*_h} \|_{L^p(\Omega)} \leq \text{const}$, where $p \in [1, \infty)$.

Then there exists $w \in W^{1,p}(\Omega)$ such that

- $w^{\mathcal{X}_h} = \frac{1}{d} w^{m_h} + \frac{d-1}{d} w^{m^*_h}$ converges to $w$ strongly in $L^p(\Omega)$
- $\nabla^{\mathcal{X}_h} w^{\mathcal{X}_h}$ converges to $\nabla w$ weakly in $L^p(\Omega)$. 
Proposition (Asymptotic $W^{1,p}$ compactness)

Assume $(w^{\Xi_h})_{h \downarrow 0}$ is a sequence of discrete functions on DDFV meshes $\Xi_h$ such that

$$\| \nabla^{\Xi_h} w^{\Xi_h} \|_{L^p(\Omega)} := \sum_{D \in \Xi_h} m_D | \nabla_D w^{\Xi_h} |^p \leq \text{const},$$

and also $\| w^{m_h} \|_{L^p(\Omega)}, \| w^{m^*_h} \|_{L^p(\Omega)} \leq \text{const}$, where $p \in [1, \infty)$.

Then there exists $w \in W^{1,p}(\Omega)$ such that

- $w^{\Xi_h} = \frac{1}{d} w^{m_h} + \frac{d-1}{d} w^{m^*_h}$ converges to $w$ strongly in $L^p(\Omega)$
- $\nabla^{\Xi_h} w^{\Xi_h}$ converges to $\nabla w$ weakly in $L^p(\Omega)$.

Proposition (Discrete Poincaré inequality)

There exists a constant $C$ independent of $h$ such that for all discrete function $w^{\Xi_h}$ on the DDFV mesh $\Xi_h$, for all $p \in [1, \infty)$ there holds

$$\| w^{m_h} \|_{L^p(\Omega)} \leq \text{const} \left( \| \nabla^{\Xi_h} w^{\Xi_h} \|_{L^p(\Omega)} + \frac{1}{|\Omega|} \left| \int_{\Omega} w^{m_h} \right| \right),$$

and idem for $w^{m_h}$ replaced with $w^{m^*_h}$.
DDFV Scheme for the Model Problem
Now we are in a position to write the scheme(s): given a family of DDFV meshes $\mathcal{T}_h$ and of time steps $\Delta t$ (such that $\Delta t \downarrow 0$ and $h = \text{size}(\mathcal{T}_h) \downarrow 0$)

$$
\begin{align*}
\text{find } & \left( (u_{i}^{\mathcal{T},n+1}, u_{e}^{\mathcal{T},n+1}, v^{\mathcal{T},n+1}) \right)_{n=0,\ldots,N} \subset (R^{\mathcal{T}})^3, N \approx T/\Delta t, \text{ satisfying} \\
& \\
& \left\{ \\
& \quad \frac{v^{\mathcal{T},n+1} - v^{\mathcal{T},n}}{\Delta t} - \text{div}^{\mathcal{T}} [M_{i}^{\mathcal{T}} \nabla^{\mathcal{T}} u_{i}^{\mathcal{T},n+1}] + (h(v^{\mathcal{T},??}))^{\mathcal{T},n+1} = I_{\text{app}}^{\mathcal{T},n+1}, \\
& \quad \frac{v^{\mathcal{T},n+1} - v^{\mathcal{T},n}}{\Delta t} + \text{div}^{\mathcal{T}} [M_{e}^{\mathcal{T}} \nabla^{\mathcal{T}} u_{e}^{\mathcal{T},n+1}] + (h(v^{\mathcal{T},??}))^{\mathcal{T},n+1} = I_{\text{app}}^{\mathcal{T},n+1}, \\
& \quad v^{\mathcal{T},n+1} = u_{i}^{\mathcal{T},n+1} - u_{e}^{\mathcal{T},n+1}, \quad v^{\mathcal{T},0} = v_{0}^{\mathcal{T}}.
\right. \\
\end{align*}
$$

Here the ionic current discretization term $(h(v^{\mathcal{T},??}))^{\mathcal{T},n+1}$ should be precised.
DDFV Scheme for the model problem

Now we are in a position to write the scheme(s): given a family of DDFV meshes $\mathcal{I}_h$ and of time steps $\Delta t$ (such that $\Delta t \downarrow 0$ and $h = \text{size}(\mathcal{I}_h) \downarrow 0$)

\[
\begin{aligned}
\text{find } \left( (u_{i}^{\mathfrak{t},n+1}, u_{e}^{\mathfrak{t},n+1}, v^{\mathfrak{t},n+1}) \right)_{n=0,\ldots,N} \subset (R^{\mathfrak{t}})^3, N \approx T/\Delta t, \text{ satisfying } \\
\frac{v^{\mathfrak{t},n+1} - v^{\mathfrak{t},n}}{\Delta t} - \text{div}^{\mathfrak{t}} \left[ M_{i}^{\mathfrak{t}} \nabla^{\mathfrak{t}} u_{i}^{\mathfrak{t},n+1} \right] + (h(v^{\mathfrak{t},??}))^{\mathfrak{t},n+1} = I_{\text{app}}^{\mathfrak{t},n+1}, \\
\frac{v^{\mathfrak{t},n+1} - v^{\mathfrak{t},n}}{\Delta t} + \text{div}^{\mathfrak{t}} \left[ M_{e}^{\mathfrak{t}} \nabla^{\mathfrak{t}} u_{e}^{\mathfrak{t},n+1} \right] + (h(v^{\mathfrak{t},??}))^{\mathfrak{t},n+1} = I_{\text{app}}^{\mathfrak{t},n+1}, \\
v^{\mathfrak{t},n+1} = u_{i}^{\mathfrak{t},n+1} - u_{e}^{\mathfrak{t},n+1}, \quad v^{\mathfrak{t},0} = v_{0}^{\mathfrak{t}}.
\end{aligned}
\]

Here the ionic current discretization term $(h(v^{\mathfrak{t},??}))^{\mathfrak{t},n+1}$ should be precised.

– for the time-implicit scheme,
we take for the value in a volume (e.g., in a primal volume $\kappa$) the expression

\[
\frac{1}{m_{\kappa}} \int_{\kappa} h(v^{\mathfrak{t},n+1}), \quad \text{i.e., } \frac{1}{m_{\kappa}} \sum_{\kappa^{*} \in \mathcal{M}^{*}} m_{\kappa \cap \kappa^{*}} \int_{\kappa^{*}} h\left(\frac{1}{3} v_{\kappa}^{n+1} + \frac{2}{3} v_{\kappa^{*}}^{n+1}\right)
\]
DDFV Scheme for the model problem

Now we are in a position to write the scheme(s): given a family of DDFV meshes $\mathcal{T}_h$ and of time steps $\Delta t$ (such that $\Delta t \downarrow 0$ and $h = \text{size}(\mathcal{T}_h) \downarrow 0$)

$$\begin{align*}
\text{find } (u_i^{\varepsilon,n+1}, u_e^{\varepsilon,n+1}, v^{\varepsilon,n+1})_{n=0,\ldots,N} \subset (R^\varepsilon)^3, N \approx T/\Delta t, \text{ satisfying }

&\quad \frac{v^{\varepsilon,n+1} - v^{\varepsilon,n}}{\Delta t} - \text{div} \varepsilon [M_i^{\varepsilon} \nabla u_i^{\varepsilon,n+1}] + (h(v^{\varepsilon,??}))^{\varepsilon,n+1} = l^{\varepsilon,n+1}_\text{app}, \\
&\quad \frac{v^{\varepsilon,n+1} - v^{\varepsilon,n}}{\Delta t} + \text{div} \varepsilon [M_e^{\varepsilon} \nabla u_e^{\varepsilon,n+1}] + (h(v^{\varepsilon,??}))^{\varepsilon,n+1} = l^{\varepsilon,n+1}_\text{app}, \\
&\quad v^{\varepsilon,n+1} = u_i^{\varepsilon,n+1} - u_e^{\varepsilon,n+1}, \quad v^{\varepsilon,0} = v_0^{\varepsilon}.
\end{align*}$$

Here the ionic current discretization term $(h(v^{\varepsilon,??}))^{\varepsilon,n+1}$ should be precised.

– for the time-implicit scheme, we take for the value in a volume (e.g., in a primal volume $\kappa$) the expression

$$\frac{1}{m_\kappa} \int_{K} h(v^{\varepsilon,n+1}), \quad \text{i.e.,} \quad \frac{1}{m_\kappa} \sum_{K^* \in \mathcal{M}^*} m_{\kappa \cap K^*} h(\frac{1}{3}v^{n+1}_\kappa + \frac{2}{3}v^{n+1}_{K^*})$$

– for the linearized implicit scheme, we write $h(z) = b(z)z - Lz - l$ and take

$$\frac{1}{m_\kappa} \int_{K} (b(v^{\varepsilon,n})v^{\varepsilon,n+1} - Lv^{\varepsilon,n+1} - l), \quad \text{with analogous interpretation.}$$
The variational nature of the time-implicit scheme

It is straightforward to check that the scheme derives from a convex coercive functional. At each time step, we have to solve the optimization problem:

\[ \text{find } \min_{\mathbb{R}^3 \times \mathbb{R}^3} J^{\bar{x},n+1}, \quad \text{where (given } v^{\bar{x},n}) \]

\[ J^{n+1}(u_i^{\bar{x}}, u_e^{\bar{x}}) := \frac{1}{2} \left[ u_i^{\bar{x}} - u_e^{\bar{x}}, u_i^{\bar{x}} - u_e^{\bar{x}} \right] - \left[ u_i^{\bar{x}} - u_e^{\bar{x}}, v^{\bar{x},n} \right] \]

\[ + \frac{\Delta t}{2} \left\{ \begin{align*}
\{ M_i \nabla^{\bar{x}} u_i^{\bar{x}}, \nabla^{\bar{x}} u_i^{\bar{x}} \} \\
\{ M_e \nabla^{\bar{x}} u_e^{\bar{x}}, \nabla^{\bar{x}} u_e^{\bar{x}} \}
\end{align*} \right\} + \frac{\Delta t}{2} \sum_{K \in \mathcal{M}, \ k^* \in \mathcal{M}^*} m_{K \cap K^*} H \left( \frac{1}{3} (u_{i,K} - u_{e,K}) + \frac{2}{3} (u_{i,K^*} - u_{e,K^*}) \right); \]

recall that \( H \) is a primitive of \( h \), \( H : z \mapsto \int_0^z h(s) \, ds \).
CONVERGENCE ANALYSIS
Convergence: the time-implicit scheme

The convergence analysis follows closely the proof of existence (e.g., by the Galerkin method) for the continuous problem \((Prob)\).
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- **Existence of a discrete solution** comes e.g. from the aforementioned convex optimization formulation. **Uniqueness** is straightforward (due to the choice of the “structure-preserving” \((h(v)\)\) discretization.)
Convergence: the time-implicit scheme

The convergence analysis follows closely the proof of existence (e.g., by the Galerkin method) for the continuous problem (Prob).

- **Existence of a discrete solution** comes e.g. from the aforementioned convex optimization formulation. **Uniqueness** is straightforward (due to the choice of the “structure-preserving” \( (h(v^T))^T \) discretization.)

- **Uniform estimates** are obtained by taking \( u_i^\xi, u_e^\xi \) for the test function in the corresponding discrete equations, and by using the discrete duality property. We get the uniform bounds:
The time-implicit case

Convergence: the time-implicit scheme

The convergence analysis follows closely the proof of existence (e.g., by the Galerkin method) for the continuous problem (Prob).

- **Existence of a discrete solution** comes e.g. from the aforementioned convex optimization formulation. **Uniqueness** is straightforward (due to the choice of the “structure-preserving” \((h(v^\infty))^{\infty}\) discretization.)

- **Uniform estimates** are obtained by taking \(u^\infty_i\), \(u^\infty_e\) for the test function in the corresponding discrete equations, and by using the discrete duality property. We get the uniform bounds:
  - on \([v^\infty,n+1, v^\infty,n+1]\), uniformly in \(h, \Delta t\) and in \(n\);
Convergence : the time-implicit scheme

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- **Existence of a discrete solution** comes e.g. from the aforementioned convex optimization formulation. **Uniqueness** is straightforward (due to the choice of the “structure-preserving” \( h(\bar{v}^t) \bar{v}^t \) discretization.)

- **Uniform estimates** are obtained by taking \( u_i^\bar{v}, u_e^\bar{v} \) for the test function in the corresponding discrete equations, and by using the discrete duality property. We get the uniform bounds :
  
  - on \( \left[ v^\bar{v}, n+1, v^\bar{v}, n+1 \right] \), uniformly in \( h, \Delta t \) and in \( n \);
  
  - on \( \sum_n \Delta t \left[ (h(v^\bar{v}, n+1))^{\bar{v}}, n+1, v^\bar{v}, n+1 \right], \) which amounts to a bound on

\[
\sum_n \Delta t \sum_{K, K^*} m_{K \cap K^*} h(\frac{1}{3}v_{K}^{n+1} + \frac{2}{3}v_{K^*}^{n+1}) (\frac{1}{3}v_{K}^{n+1} + \frac{2}{3}v_{K^*}^{n+1}) \equiv \int\int_{Q_T} h(v^{\bar{v}, \Delta t}) v^{\bar{v}, \Delta t};
\]

this yields a uniform \( L^r \) estimate on \( v^{\bar{v}, \Delta t} \), due to the assumptions on \( h \).
Convergence: the time-implicit scheme

The convergence analysis follows closely the proof of existence (e.g., by the Galerkin method) for the continuous problem $(Prob)$.

- **Existence of a discrete solution** comes e.g. from the aforementioned convex optimization formulation. **Uniqueness** is straightforward (due to the choice of the “structure-preserving” $(h(v^\bar{x}))^\bar{x}$ discretization.)

- **Uniform estimates** are obtained by taking $u^\bar{x}_i, u^\bar{x}_e$ for the test function in the corresponding discrete equations, and by using the discrete duality property. We get the uniform bounds:
  
  - on $[v^\bar{x}, n+1, v^\bar{x}, n+1]$, uniformly in $h, \Delta t$ and in $n$;
  
  - on $\sum_n \Delta t \left[ (h(v^\bar{x}, n+1))^{\bar{x}}, n+1, v^\bar{x}, n+1 \right]$, which amounts to a bound on

  $\sum_n \Delta t \sum_{K, K^*} m_{K \cap K^*} h(\frac{1}{3} v^{n+1}_K + \frac{2}{3} v^{n+1}_{K^*}) (\frac{1}{3} v^{n+1}_K + \frac{2}{3} v^{n+1}_{K^*}) \equiv \iiint_{Q_T} h(v^\bar{x}, \Delta t) v^\bar{x}, \Delta t$;

  this yields a uniform $L^r$ estimate on $v^\bar{x}, \Delta t$, due to the assumptions on $h$.

  - on $\sum_n \Delta t \left\{ M^\bar{x}_{i, e} \nabla^\bar{x} u^\bar{x}_{i, e}, n+1, \nabla^\bar{x} u^\bar{x}_{i, e}, n+1 \right\}$, which implies the $L^2$ estimate on $\nabla^\bar{x} u^\bar{x}_{i, e}, \Delta t$ and on the space translates of both $v^m, \Delta t, v^m^*, \Delta t$.
The time-implicit case

**Convergence : the time-implicit scheme**

The convergence analysis follows closely the proof of existence (e.g., by the Galerkin method) for the continuous problem \((\text{Prob})\).

- **Existence of a discrete solution** comes e.g. from the aforementioned convex optimization formulation. **Uniqueness** is straightforward (due to the choice of the “structure-preserving” \((h(v^\xi))^\xi\) discretization.)

**Uniform estimates** are obtained by taking \(u_i^\xi, u_e^\xi\) for the test function in the corresponding discrete equations, and by using the discrete duality property. We get the uniform bounds:

- on \([v^\xi,n+1, v^\xi,n+1]\), uniformly in \(h, \Delta t\) and in \(n\);
- on \(\sum_n \Delta t [(h(v^\xi,n+1))^\xi,n+1, v^\xi,n+1]\), which amounts to a bound on

\[
\sum_n \Delta t \sum_{K \cap K^*} m_{K \cap K^*} h(\frac{1}{3} v_{K}^{n+1} + \frac{2}{3} v_{K^*}^{n+1}) (\frac{1}{3} v_{K}^{n+1} + \frac{2}{3} v_{K^*}^{n+1}) \equiv \iint_{Q_T} h(v^\xi,\Delta t)v^\xi,\Delta t;
\]

this yields a uniform \(L^r\) estimate on \(v^\xi,\Delta t\), due to the assumptions on \(h\).

- on \(\sum_n \Delta t \left\{ \nabla^\xi u_{i,e}^\xi, n+1, \nabla^\xi u_{i,e}^\xi, n+1 \right\}\), which implies the \(L^2\) estimate on \(\nabla^\xi u_{i,e}^\xi,\Delta t\) and on the space translates of both \(v^m,\Delta t, v^m,^*,\Delta t\);

- on the \(L^2\) time translates of \(v^m,\Delta t, v^m,^*,\Delta t\), thanks to the previous estimates and the “evolution nature” of the problem.
The time-implicit case

Convergence: the time-implicit scheme (cont^d)

The above estimates allow to use the compactness arguments and deduce that, up to extraction of a subsequence:
The time-implicit case

Convergence: the time-implicit scheme (cont’d)

The above estimates allow to use the compactness arguments and deduce that, up to extraction of a subsequence:

- $u_{i,e}^{\xi,\Delta t}$ converge to some limits $u_{i,e}$ in $L^2(0,T;H^1(\Omega))$ weakly;
- $v^{\xi,\Delta t}$ converges to $v := u_i - u_e$ in $L^2(Q_T)$ strongly and in $L^r(Q_T)$ weakly;
- the discrete ionic current term $(h(v^{\xi,\Delta t}))^{\xi}$ converges to some limit $\chi$ in $L^{r'}(Q_T)$ weakly ($\chi$ cannot yet be recognized as $h(v)$).
The time-implicit case

Convergence : the time-implicit scheme (cont’d)

- The above estimates allow to use the compactness arguments and deduce that, up to extraction of a subsequence:
  - $u^{\xi, \Delta t}_{i,e}$ converge to some limits $u_{i,e}$ in $L^2(0, T; H^1(\Omega))$ weakly;
  - $v^{\xi, \Delta t}$ converges to $v := u_i - u_e$ in $L^2(Q_T)$ strongly and in $L^r(Q_T)$ weakly;
  - the discrete ionic current term $\left( h(v^{\xi, \Delta t}) \right)^{\xi}$ converges to some limit $\chi$ in $L^{r'}(Q_T)$ weakly ($\chi$ cannot yet be recognized as $h(v)$).

- We take a smooth test function $\varphi$, project it on the mesh to get $\varphi^{\xi, \Delta t}$, and take it for the test function in the scheme. The discrete duality and simple rearrangements yield (for the first eqn of the system)

\[
- \sum_n \Delta t \left[ \nabla \varphi^{\xi, n+1} - \nabla \varphi^{\xi, n} \frac{\Delta t}{\Delta t} \right] + \sum_n \left\{ \sum_{K \cap K^*} m_{K \cap K^*} h \left( \frac{1}{3} v^{n+1}_K + \frac{2}{3} v^{n+1}_{K^*} \right) \left( \frac{1}{3} \varphi^{n+1}_K + \frac{2}{3} \varphi^{n+1}_{K^*} \right) \right\}
\]

\[
+ \sum_n \Delta t \sum_{K, K^*} m_{K \cap K^*} h \left( \frac{1}{3} v^{n+1}_K + \frac{2}{3} v^{n+1}_{K^*} \right) \left( \frac{1}{3} \varphi^{n+1}_K + \frac{2}{3} \varphi^{n+1}_{K^*} \right)
\]

\[
= \sum_n \Delta t \left[ I^{\xi, n+1}_{app}, \varphi^{\xi, n+1} \right] + \left[ v^{\xi, 0}, \varphi^{\xi, 0} \right].
\]
The time-implicit case

Convergence: the time-implicit scheme (cont’d)

Replacing $\varphi^{x, \Delta t}$ by $\varphi$, replacing $\nabla^{x} \varphi^{x, \Delta t}$ with $\nabla \varphi$, etc., we can write the “continuous form of the discrete equations”:

$$\iint_{Q_T} \left( -v^{x, \Delta t} \partial_t \varphi + (M_i^{x} \nabla u_i) \cdot \nabla \varphi + h(v^{x, \Delta t}) \varphi^{x, \Delta t} - I_{app} \varphi \right) = \int_{\Omega} v_0 \varphi(0) + Rem$$

where the remainder terms $Rem \equiv Rem(\phi, h, \Delta t)$ converge to zero as $h, \Delta t \downarrow 0$ thanks to the consistency of $\nabla^{x}$ and to the previously stated uniform estimates on discrete solutions.
The time-implicit case

Convergence : the time-implicit scheme (cont\textsuperscript{d})

Replacing $\varphi^\tau,\Delta t$ by $\varphi$, replacing $\nabla^\tau \varphi^\tau,\Delta t$ with $\nabla \varphi$, etc., we can write the “continuous form of the discrete equations”:

\[
\int\int_{Q_T} \left( -v^\tau,\Delta t \partial_t \varphi + (M^\tau_i \nabla u_i) \cdot \nabla \varphi + h(v^\tau,\Delta t)\varphi^\tau,\Delta t - I_{\text{app}} \varphi \right) = \int_{\Omega} v_0 \varphi(0) + Rem
\]

where the remainder terms $Rem \equiv Rem(\varphi, h, \Delta t)$ converge to zero as $h, \Delta t \downarrow 0$ thanks to the consistency of $\nabla^\tau$ and to the previously stated uniform estimates on discrete solutions.

Passing to the limit as $h, \Delta t \downarrow 0$ in the above equation (using the aforementioned compactnesses), we get

\[
\partial_t v - \text{div} \left( M_i(x) \nabla u_i \right) + \chi = I_{\text{app}}, \quad v(0) = v_0 \quad \text{in } D'(\mathbb{R} \times \Omega)
\]

It remains to identify $\chi$ to $h(v)$, which is done by the classical monotonicity argument (Minty-Browder).
The time-implicit case

**Convergence : the time-implicit scheme (cont^d)**

- Replacing \( \varphi^{\tau, \Delta t} \) by \( \varphi \), replacing \( \nabla^{\tau} \varphi^{\tau, \Delta t} \) with \( \nabla \varphi \), etc., we can write the "continuous form of the discrete equations" :

\[
\iint_{Q_T} \left( -v^{\tau, \Delta t} \partial_t \varphi + (M_i^{\tau} \nabla u_i) \cdot \nabla \varphi + h(v^{\tau, \Delta t})\varphi^{\tau, \Delta t} - I_{app} \varphi \right) = \int_{\Omega} v_0 \varphi(0) + \text{Rem}
\]

where the remainder terms \( \text{Rem} \equiv \text{Rem}(\varphi, h, \Delta t) \) converge to zero as \( h, \Delta t \downarrow 0 \) thanks to the consistency of \( \nabla^{\tau} \) and to the previously stated uniform estimates on discrete solutions.

- Passing to the limit as \( h, \Delta t \downarrow 0 \) in the above equation (using the aforementioned compactnesses), we get

\[
\partial_t \nu - \text{div} (M_i(x) \nabla u_i) + \chi = I_{app}, \quad \nu(0) = v_0 \quad \text{in } \mathcal{D}'([0, T] \times \Omega)
\]

- It remains to identify \( \chi \) to \( h(\nu) \), which is done by the classical monotonicity argument (Minty-Browder).

- As a byproduct, we get strong \( L^2 \) convergence of \( \nabla^{\tau} u_{i,e}^{\tau, \Delta t} \) to \( \nabla u_{i,e} \), the strong \( L^r \) convergence of \( v^{\tau, \Delta t} \) to \( \nu \), and the strong \( L^{r'} \) convergence of \( (h(v^{\tau, \Delta t}))^{\tau} \) to \( h(\nu) \).

- Uniqueness for \((\text{Prob}) \implies \) all the sequence of the DDFV approximation converges (strongly !) to the unique solution of \((\text{Prob})\).
Convergence: the linearized implicit scheme

The only supplementary difficulty for the analysis of the linearized implicit scheme lies in obtaining the uniform estimate on $v^{\Xi, \Delta t}$ in $L^r(Q_T)$.

More exactly, we need at least an $L^1$ weak compactness estimate on the ionic current term.
The linearized implicit case

Convergence: the linearized implicit scheme

The only supplementary difficulty for the analysis of the linearized implicit scheme lies in obtaining the uniform estimate on $v^{\xi,\Delta t}$ in $L^r(Q_T)$.

More exactly, we need at least an $L^1$ weak compactness estimate on the ionic current term. Fortunately,

- The scheme is designed in such a way that it gives a uniform estimate on
  \[
  \int_0^T \int_{Q_T} b(v^{\xi,\Delta t}|_{(t-\Delta t,x)}) |v^{\xi,\Delta t}|_{(t,x)}^2 \, dt \, dx.
  \]
  where $b(z) := (h(z) + Lz + l)/z \geq 0$, by the assumptions on $h$.
- Recall that we also have a uniform $L^2(Q_T)$ bound on $v^{\xi,\Delta t}$. 
The linearized implicit case

**Convergence : the linearized implicit scheme**

The only supplementary difficulty for the analysis of the linearized implicit scheme lies in obtaining the uniform estimate on \( v^{\bar{x},\Delta t} \) in \( L^r(Q_T) \).

More exactly, we need at least an \( L^1 \) weak compactness estimate on the ionic current term. Fortunately,

- The scheme is designed in such a way that it gives a uniform estimate on

\[
\int_Q \int_{Q_T} b(v^{\bar{x},\Delta t}|_{(t-\Delta t,x)}) \, |v^{\bar{x},\Delta t}|_{(t,x)}^2 \, dtdx.
\]

where \( b(z) := (h(z) + Lz + l)/z \) is \( \geq 0 \), by the assumptions on \( h \).
- Recall that we also have a uniform \( L^2(Q_T) \) bound on \( v^{\bar{x},\Delta t} \).
- Notice that the assumption \( r < 4 \) yields \( 0 \leq b(z) \ll z^2 \) for \( |z| \gg 1 \).

This allows to deduce an equi-integrability estimate on the ionic current term (which is, essentially, \( b(v^{\bar{x},n}) v^{\bar{x},n+1} \)) from the decomposition

\[
\forall \alpha \quad |b(v^{\bar{x},n}) v^{\bar{x},n+1}| \leq \alpha b(v^{\bar{x},n}) + \frac{1}{\alpha} b(v^{\bar{x},n}) |v^{\bar{x},n+1}|^2.
\]

This trick allows to bypass the difficulty and conclude the convergence proof also for the linearized implicit scheme.
The linearized implicit case

Merci !