



**HAL**  
open science

# Approximated lax pairs and empirical interpolation for nonlinear parabolic partial differential equations

Jean-Frédéric Gerbeau, Damiano Lombardi, Elisa Schenone

► **To cite this version:**

Jean-Frédéric Gerbeau, Damiano Lombardi, Elisa Schenone. Approximated lax pairs and empirical interpolation for nonlinear parabolic partial differential equations . 2016. hal-01278778

**HAL Id: hal-01278778**

**<https://inria.hal.science/hal-01278778>**

Preprint submitted on 24 Feb 2016

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# APPROXIMATED LAX PAIRS AND EMPIRICAL INTERPOLATION FOR NONLINEAR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

JEAN-FRÉDÉRIC GERBEAU\*<sup>†</sup> DAMIANO LOMBARDI\*<sup>†</sup> ELISA SCHENONE\*<sup>†</sup>

**1. Introduction.** Several methods exist to approximate the solutions of PDEs with a reduced number of degrees of freedom (Reduced Basis Methods, Proper Orthogonal Decomposition, *etc.*). But time-dependent problems dominated by transport or propagation phenomena remain a challenge for reduced-order modelling.

In [6], a new approach was proposed to approximate the nonlinear evolution partial differential equations. This method, called ALP, is based on approximations of generalized Lax pairs. Contrary to other reduced-order methods, it is not based on an off-line / on-line strategy, and the basis on which the solution is searched for evolves in time according to a dynamics specific to the problem. This algorithm was successfully used for various nonlinear problems, including the equations of cardiac electrophysiology [7], which exhibit front propagation. Two weaknesses of the original method were the limitation to polynomial nonlinearities and a complexity proportional to the power three of the number of modes. In this article, a new algorithm is proposed which does not suffer from these two shortcomings.

The ALP-EI method introduced in this work combines the idea of ALP, i.e. a time evolving basis which does not rely on a database, and the treatment of nonlinear terms using a selection of spatial points from an Empirical Interpolation technique in the same spirit as in [1, 3]. More specifically, the definition of the basis functions and of their time evolution does not change compared to the ALP method, but the functions and the operator used to solve the reduced order problem are evaluated on a finite set of points which is typically a small subset of the finite element nodes. As a consequence, the ALP-EI method is well-suited to non-polynomial nonlinearities, and much less expensive than the original ALP method.

**2. The ALP-EI method.** Let  $\Omega$  be a bounded subset of  $\mathbb{R}^d$ , with  $d = 1, 2$  or  $3$ , and  $T > 0$ . We consider a parabolic nonlinear partial differential equation (PDE):

$$(2.1) \quad \begin{cases} \frac{\partial u}{\partial t} - \Delta u = f(u), & \text{in } \Omega \times (0, T), \\ \frac{\partial u}{\partial n} = 0, & \text{on } \partial\Omega \times (0, T), \\ u(0) = u_0, & \text{in } \Omega. \end{cases}$$

The nonlinear function  $f$  and the initial data  $u_0$  are assumed to have a regularity sufficient to give a sense to all the formal computations hereafter.

**2.1. The ALP method in a nutshell.** In this Section, we briefly recall the main ideas of the Approximated Lax Pair (ALP) method proposed in [6]. In the ALP algorithm, the solution of the PDE (2.1) is approximated by an expansion on a time dependent basis:

$$(2.2) \quad u(x, t) \simeq \sum_{i=1}^{N_M} \beta_i(t) \varphi_i(x, t).$$

---

\*Inria, 2 rue simone Iff, 75012 Paris, France.

<sup>†</sup>Sorbonne Universités UPMC, UMR 7598 LJLL, 75005 Paris, France.

The basis is made of eigenmodes defined by:

$$(2.3) \quad \mathcal{L}(u(x, t))\varphi_i(x, t) = \lambda_i(t)\varphi_i(x, t),$$

where  $\mathcal{L}(u)$  is a linear Schrödinger operator:

$$(2.4) \quad \mathcal{L}(u)\varphi := -\Delta\varphi - \chi u\varphi,$$

where  $\chi$  is a given positive parameter. The eigenmodes are solutions of an evolution equations:

$$(2.5) \quad \partial_t\varphi_i = \mathcal{M}(u)\varphi_i.$$

The ALP method relies on the observation that, in many situations, the solution  $u$  can be economically represented with a few modes defined by (2.3). If an approximation of (2.5) is available, then the eigenvalue problem has to be solved only once, and the modes can be propagated in time.

For some problems, like the Korteweg - de Vries equation, a closed form of  $\mathcal{M}(u)$  can be obtained such that the Lax equation

$$(2.6) \quad \partial_t\mathcal{L}(u) + \mathcal{L}(u)\mathcal{M}(u) - \mathcal{M}(u)\mathcal{L}(u) = 0$$

is satisfied when  $u$  is solution to (2.1). In such a case, the eigenvalues  $\lambda_i$  have the remarkable property to be constant in time, which provides first integrals of the dynamics, and the operators  $\mathcal{L}(u)$  and  $\mathcal{M}(u)$  are known as Lax pairs [9]. In general, the closed form of  $\mathcal{M}(u)$  is unknown and/or the eigenvalues are not constant. In these cases, approximations of  $\mathcal{M}(u)$  and of the equation satisfied by the eigenvalues were proposed in [6]. The approximation was based on a  $L^2$  projection of the equations on the eigenmodes. To avoid the shortcomings recalled in the introduction, we propose another strategy in the following.

**2.2. Finite element formulation of the Approximated Lax Pair.** From now, the “full-order model” refers to the approximation of (2.1) on a finite dimensional space  $V$  constructed with continuous piecewise affine functions. The quantities  $\varphi, u, \mathcal{L}, \mathcal{M}, \dots$  used in the previous section now denote their finite element counterpart. The finite element basis of  $V$  is denoted by  $(v_1, \dots, v_{\mathcal{N}})$ . The solution  $u(x, t) = \sum_{i=1}^{\mathcal{N}} u_i(t)v_i(x) \in V$  of the full-order model is such that for  $i = 1, \dots, \mathcal{N}$ ,

$$(2.7) \quad \int_{\Omega} \partial_t uv_i + \int_{\Omega} \nabla u \cdot \nabla v_i = \int_{\Omega} f(u)v_i.$$

The finite element approximation of the eigenmodes of (2.3) is given by:

$$\varphi_k(x, t) = \sum_{j=1}^{\mathcal{N}} \Phi_{jk}(t)v_j(x), \quad \text{for } k = 1, \dots, N_M.$$

The vector  $\Phi_k(t) \in \mathbb{R}^{\mathcal{N}}$  denotes the components of  $\varphi_k(x, t)$  on the finite element basis:  $\Phi_k(t) = (\Phi_{jk}(t))_{j=1 \dots \mathcal{N}}$ . The following  $\mathcal{N} \times \mathcal{N}$  matrices are defined:

$$\mathcal{L}(u) = \left[ \int_{\Omega} \nabla v_j \cdot \nabla v_i - \chi \int_{\Omega} uv_j v_i \right]_{i,j=1 \dots \mathcal{N}}, \quad \partial_t \mathcal{L}(u) = \left[ -\chi \int_{\Omega} \partial_t uv_j v_i \right]_{i,j=1 \dots \mathcal{N}},$$

and the Gram (or mass) matrix  $\mathcal{G} = \left[ \int_{\Omega} v_j v_i \right]_{i,j=1 \dots \mathcal{N}}$ .

The usual Euclidian scalar product in  $\mathbb{R}^{\mathcal{N}}$  is denoted by  $\langle \cdot, \cdot \rangle$ . Another scalar product is defined in  $\mathbb{R}^{\mathcal{N}}$  by  $\langle \cdot, \cdot \rangle_{\mathcal{G}} = \langle \mathcal{G} \cdot, \cdot \rangle$ . With this notation,  $\int_{\Omega} \varphi_k \varphi_l = \langle \Phi_k, \Phi_l \rangle_{\mathcal{G}}$ .

The vectors  $\Phi_k(t)$  satisfy

$$(2.8) \quad \mathcal{L}(u(t))\Phi_k(t) = \lambda_k(t)\mathcal{G}\Phi_k(t),$$

and are normalized such that  $\langle \Phi_k, \Phi_l \rangle_{\mathcal{G}} = \delta_{kl}$ , where  $\delta_{kl}$  is the Kronecker delta.

Let  $M$  be the  $N_M \times N_M$  skew-symmetric matrix  $M$  defined by:

$$(2.9) \quad M_{kl} = \langle \partial_t \Phi_l, \Phi_k \rangle_{\mathcal{G}}.$$

**PROPOSITION 2.1.** *Let  $u$  be the solution of (2.7). Let  $\Phi_k(t)$  be the eigenmodes and  $\lambda_k(t)$  the eigenvalues defined by (2.8). Then*

$$(2.10) \quad \partial_t \lambda_k = -\chi \int_{\Omega} \partial_t u \varphi_k^2.$$

Let  $M$  be the matrix defined by (2.9). If  $k$  and  $l$  are such that  $\lambda_k \neq \lambda_l$ , then

$$(2.11) \quad M_{kl} = \frac{\chi}{\lambda_k - \lambda_l} \int_{\Omega} \partial_t u \varphi_k \varphi_l.$$

*Proof.* The time derivative of (2.8) gives:

$$(2.12) \quad \partial_t \mathcal{L}(u)\Phi_k + (\mathcal{L}(u) - \lambda_k \mathcal{G})\partial_t \Phi_k = \partial_t \lambda_k \mathcal{G}\Phi_k$$

Taking the scalar product with  $\Phi_l$  and using the symmetry of the matrix  $\mathcal{L}(u)$ ,

$$\langle \partial_t \mathcal{L}(u)\Phi_k, \Phi_l \rangle + (\lambda_l - \lambda_k)\langle \mathcal{G}\partial_t \Phi_k, \Phi_l \rangle = \partial_t \lambda_k \langle \mathcal{G}\Phi_k, \Phi_l \rangle,$$

Thus

$$(\lambda_l - \lambda_k)M_{lk} = \partial_t \lambda_k \delta_{kl} + \chi \int_{\Omega} \partial_t u \varphi_k \varphi_l,$$

hence the result.  $\square$

*Remark 2.1.* Denoting by  $\mathcal{M}(u)$  the matrix such that  $\partial_t \Phi_k = \mathcal{M}(u)\Phi_k$ , relation (2.12) reads:

$$\partial_t \mathcal{L}(u)\Phi_k + \mathcal{L}(u)\mathcal{M}(u)\Phi_k - \mathcal{M}(u)\mathcal{L}(u)\Phi_k = \partial_t \lambda_k \Phi_k$$

which is a discrete counterpart of the Lax equation (2.6) in the non-isospectral case. But the matrix  $\mathcal{M}(u)$  being not explicitly known, this relation is of no practical use in this form. Matrix  $M$  defined by (2.9) can be viewed as an approximation of  $\mathcal{M}(u)$  since  $M_{kl} = \langle \mathcal{M}(u)\Phi_l, \Phi_k \rangle_{\mathcal{G}}$ .

*Remark 2.2.* Consider the equation:

$$(\lambda_l - \lambda_k)M_{lk} = \partial_t \lambda_k \delta_{kl} + \chi \int_{\Omega} \partial_t u \varphi_k \varphi_l,$$

When  $l \neq k$ , but  $\lambda_l = \lambda_k$ , i.e. when there is a degenerate eigenvalue (multiplicity greater than one), there is an orthogonal transformation invariant subspace spanned by the corresponding eigenfunctions, and the equation for  $M_{lk}$  does no longer make sense. The resolution of this degeneracy is a classical result in the perturbation theory in quantum mechanics. In particular, when  $\lambda_l = \lambda_k$ , the evolution representation reads:  $\langle \partial_t \varphi_l, \varphi_k \rangle = 0$ . The fact that the eigenfunctions are defined up to a transformation can be used to solve this equation. Let us consider the sub-matrix whose entries are  $S_{ij} = \langle \partial_t u \varphi_l, \varphi_k \rangle$ , for the indices corresponding to  $\lambda_l = \lambda_k$ . The eigenvectors of  $S$  define a linear combination of the eigenfunctions such that the evolution operator representation is zero. When using this linear combination to update the eigenfunction, we obtain that the eigenvalue crossing results in a "jump" of the eigenfunctions.

*Remark 2.3.* In the original ALP method,  $\partial_t u$  was approximated by an expansion  $\sum_{i=1}^{N_M} \gamma_i \varphi_i$  and the quantity  $\int_{\Omega} \partial_t u \varphi_k \varphi_l$  in (2.10) and (2.11) was approximated by  $\sum_{i=1}^{N_M} \gamma_i \int_{\Omega} \varphi_i \varphi_k \varphi_l$ . The third order tensor  $[\int_{\Omega} \varphi_i \varphi_k \varphi_l]$  had to be propagated (see Section 3.3 of [6]), which could be costly when the number of mode  $N_M$  was high. Besides, to relate the components  $\gamma_i$  of  $\partial_t u$  to the components  $\beta_i$  of  $u$ , the nonlinearity of  $f(u)$  was supposed to be polynomial.

**2.3. Approximation of the finite element formulation.** In this section we derive an approximation of the quantity  $\int_{\Omega} \partial_t u \varphi_k \varphi_l$ , which appears in the expression of (2.10) and (2.11). For  $k = 1, \dots, N_M$ , the evolution of the eigenvector  $\Phi_k$  is approximated by:

$$(2.13) \quad \partial_t \tilde{\Phi}_k = \tilde{M} \tilde{\Phi}_k.$$

where  $\tilde{M}$  will be defined below. An approximation  $\tilde{U}(t) \in \mathbb{R}^N$  of the degrees of freedom of the solution  $u(\cdot, t) \in V$  is searched for as an expansion on the eigenvectors:

$$(2.14) \quad \tilde{U}(t) = \sum_{l=1}^{N_M} \beta_l(t) \tilde{\Phi}_l(t).$$

Thus we have:

$$\partial_t \tilde{U} = \sum_{l=1}^{N_M} \partial_t \beta_l \tilde{\Phi}_l + \sum_{l=1}^{N_M} \beta_l \tilde{M} \tilde{\Phi}_l,$$

and by projection on  $\tilde{\Phi}_k$ , we obtain:

$$(2.15) \quad \partial_t \beta_k + \sum_{l=1}^{N_M} \tilde{M}_{kl} \beta_l = \langle \partial_t \tilde{U}, \tilde{\Phi}_k \rangle_{\mathcal{G}}.$$

For any continuous function  $g$  defined on  $\Omega$ , we will use the following approximation repeatedly :

$$(2.16) \quad \int_{\Omega} g v_i \simeq \sum_{j=1}^{\mathcal{N}} \left( \int_{\Omega} v_j v_i \right) g_j,$$

where  $g_j$  denotes the interpolation of  $g$  at the  $j$ -th finite element nodes.

Multiplying (2.8) by  $\beta_k$  and summing over  $k$ , we obtain:

$$\mathcal{L}(u(t))\tilde{U}(t) = \sum_{k=1}^{N_M} \lambda_k(t) \beta_k(t) \mathcal{G}\tilde{\Phi}_k(t),$$

thus

$$K\tilde{U} = \chi \left[ \int_{\Omega} uv_j v_i \right]_{i,j} \tilde{U} + \sum_{k=1}^{N_M} \lambda_k \beta_k \mathcal{G}\tilde{\Phi}_k.$$

With the approximation (2.14) and (2.16), we have:

$$K\tilde{U} \simeq \chi \mathcal{G}(\tilde{U} \odot \tilde{U}) + \sum_{k=1}^{N_M} \lambda_k \beta_k \mathcal{G}\tilde{\Phi}_k,$$

where  $\odot$  denotes the Hadamard product, i.e. the element-by-element multiplication. Then using this approximation in (2.7), and again (2.14) and (2.16), we obtain:

$$\mathcal{G}\partial_t \tilde{U} + \chi \mathcal{G}(\tilde{U} \odot \tilde{U}) + \sum_{k=1}^{N_M} \lambda_k \beta_k \mathcal{G}\tilde{\Phi}_k \simeq \mathcal{G}f(\tilde{U}),$$

where  $f(\tilde{U})$  denotes the vector  $(f(\tilde{U}_j))_{j=1\dots N}$ . We therefore obtain the following approximation

$$(2.17) \quad \partial_t \tilde{U} \simeq f(\tilde{U}) - \chi \tilde{U} \odot \tilde{U} - \sum_{k=1}^{N_M} \lambda_k \beta_k \tilde{\Phi}_k.$$

Using (2.14), we have:

$$\int_{\Omega} \partial_t u \varphi_k \varphi_l \simeq \sum_{j=1}^N \left( \int_{\Omega} v_j \varphi_l \right) \partial_t \tilde{U}_j \tilde{\Phi}_{jk} = \sum_{i,j=1}^N \Phi_{il} \left( \int_{\Omega} v_j v_i \right) \partial_t \tilde{U}_j \tilde{\Phi}_{jk}.$$

Combining the last two expressions, we obtain the following approximation:

$$(2.18) \quad \int_{\Omega} \partial_t u \varphi_k \varphi_l \simeq \tilde{\Phi}_l^T \mathcal{G}(\tilde{\Phi}_k \odot \tilde{F}),$$

where  $\tilde{F} = f(\tilde{U}) - \chi \tilde{U} \odot \tilde{U} - \sum_{k=1}^{N_M} \lambda_k \beta_k \tilde{\Phi}_k$ .

Thus, we deduce from (2.10) and (2.11):

$$(2.19) \quad \partial_t \lambda_k = -\chi \int_{\Omega} \partial_t u \varphi_k^2 \approx -\chi \tilde{\Phi}_k^T \mathcal{G}(\tilde{\Phi}_k \odot \tilde{F}),$$

$$(2.20) \quad M_{kl} = \frac{\chi}{\lambda_k - \lambda_l} \int_{\Omega} \partial_t u \varphi_k \varphi_l \approx \frac{\chi}{\lambda_k - \lambda_l} \tilde{\Phi}_l^T \mathcal{G}(\tilde{\Phi}_k \odot \tilde{F}).$$

**2.4. The ALP-EI algorithm.** In the previous section, we derived the approximation (2.18), which can be used to approximate the expression (2.11) of the operator  $M$ , and the differential equation (2.10) satisfied by the eigenvalues  $\lambda_k$ . But in (2.18), the size of the vectors is the dimension  $\mathcal{N}$  of the full order space. To obtain a reduced order model, we have to further simplify this expression. To do so, we introduce  $N_P$  interpolation points, which are picked among the  $\mathcal{N}$  nodes of the finite element mesh. The choice of these points will be explained in Section 2.6. Consider the interpolation matrix

$$P = \left[ e_{p_1}, \dots, e_{p_{N_P}} \right] \in \mathbb{R}^{\mathcal{N}, N_P},$$

where  $e_{p_j} = [0, \dots, 0, 1, 0, \dots, 0]^T \in \mathbb{R}^{\mathcal{N}}$  is the  $p_j$ -th column of the identity matrix of  $\mathbb{R}^{\mathcal{N} \times \mathcal{N}}$ . For  $k = 1 \dots N_P$ , we define  $\Phi_k(0) \in \mathbb{R}^{\mathcal{N}}$  as the first  $N_P$  normalized modes solution to problem (2.8), and the vectors  $\Psi_k \in \mathbb{R}^{N_P}$  by

$$\Psi_k = P^T \Phi_k(0).$$

We denote by  $\Phi(0)$  the  $\mathcal{N} \times N_P$  matrix whose columns are the vectors  $\Phi_j(0)$ ,  $j = 1 \dots N_P$ , by  $\Psi$  the  $N_P \times N_P$  matrix whose columns are the vectors  $\Psi_j$ ,  $j = 1 \dots N_P$ , and by  $\hat{\Phi}(t)$  the  $N_P \times N_M$  matrix whose columns are the  $\hat{\Phi}_j(t)$ ,  $j = 1 \dots N_M$  (see Fig. 2.1).

We recall that the basis  $(\Phi_k(0))_{k=1 \dots N_P}$  is orthonormal with respect to the scalar product  $\langle \cdot, \cdot \rangle_{\mathcal{G}}$  defined by the Gram matrix  $\mathcal{G}$ . This is of course no longer true for the basis  $(\Psi_k)_{k=1 \dots N_P}$ . We therefore introduce a new matrix  $G \in \mathbb{R}^{N_P \times N_P}$  such that  $(\Psi_k)_{k=1 \dots N_P}$  is orthonormal for the scalar product  $\langle \cdot, \cdot \rangle_G$ , i.e.  $\Psi^T G \Psi = I$ , where  $I \in \mathbb{R}^{N_P \times N_P}$  is the identity matrix. The matrix  $\Psi$  can be QR-decomposed  $\Psi = QR$ , where  $Q$  is an orthonormal matrix and  $R$  is an upper triangular matrix, which is obtained without any extra costs when applying a modified Gram-Schmidt orthonormalization. Then, the expression of  $G$  can be obtained, offline and once for all, by

$$(2.21) \quad G = QR^{-T}R^{-1}Q^T.$$

Then we can repeat *mutatis mutandis* the derivation presented in the previous Section, the only change being that the Gram matrix  $\mathcal{G}$  is replaced by  $G$ . The interpolation  $\hat{U}(t)$  of the solution  $u(\cdot, t) \in V$  is now searched for in the space  $\mathbb{R}^{N_P}$  and its expansion on the mobile basis  $(\hat{\Phi}_l(t))_{l=1 \dots N_M}$  is given by:

$$(2.22) \quad \hat{U}(t) = \sum_{l=1}^{N_M} \hat{\beta}_l(t) \hat{\Phi}_l(t).$$

The counterpart of (2.15) is

$$\partial_t \hat{\beta}_k + \sum_{l=1}^{N_M} \hat{M}_{kl} \hat{\beta}_l = \langle \partial_t \hat{U}, \hat{\Phi}_k \rangle_G.$$

The counterpart of (2.17) is

$$\partial_t \hat{U} = f(\hat{U}) - \chi \hat{U} \odot \hat{U} - \sum_{l=1}^{N_M} \hat{\lambda}_l \hat{\beta}_l \hat{\Phi}_l := \hat{F}$$

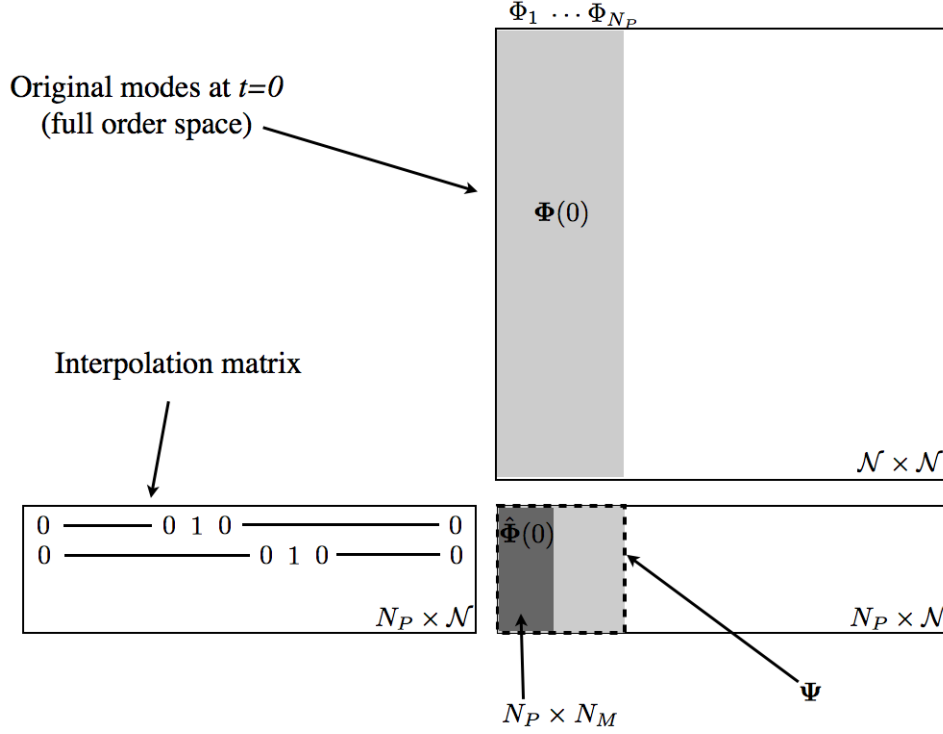


FIG. 2.1. Schematic representation of matrices  $\Phi(0)$ ,  $\Psi$  and  $\hat{\Phi}(0)$ .

And the counterparts of (2.18) and (2.19) are:

$$\partial_t \hat{\lambda}_k = -\chi \hat{\Phi}_k^T G(\hat{\Phi}_k \odot \hat{F}),$$

and

$$\hat{M}_{kl} = \frac{\chi}{\hat{\lambda}_k - \hat{\lambda}_l} \hat{\Phi}_l^T G(\hat{\Phi}_k \odot \hat{F}).$$

To summarize, for  $k = 1 \dots N_M$ ,  $\hat{\beta}_k(t)$  and  $\hat{\Phi}_k(t)$  are defined by:

$$(2.23) \quad \left\{ \begin{array}{l} \partial_t \hat{\beta}_k + \sum_{l=1}^{N_M} \hat{M}_{kl} \hat{\beta}_l = \hat{F}^T G \hat{\Phi}_k, \\ \partial_t \hat{\Phi}_k = \hat{M} \hat{\Phi}_k, \\ \partial_t \hat{\lambda}_k = -\chi \hat{\theta}_{kk}, \\ \hat{M}_{kl} = \frac{\chi}{\hat{\lambda}_k - \hat{\lambda}_l} \hat{\theta}_{kl}, \text{ if } \hat{\lambda}_k \neq \hat{\lambda}_l, \text{ and } \hat{M}_{kl} = 0 \text{ if } \hat{\lambda}_k = \hat{\lambda}_l, \\ \hat{\theta}_{kl} = \hat{\Phi}_l^T G(\hat{\Phi}_k \odot \hat{F}), \\ \hat{F} = f(\hat{U}) - \chi \hat{U} \odot \hat{U} - \sum_{l=1}^{N_M} \hat{\lambda}_l \hat{\beta}_l \hat{\Phi}_l. \end{array} \right.$$



**2.5. Reconstruction in the full order space.** The solution (2.22) obtained with the ALP-EI algorithm (2.23) only involves computations in the reduced order space. We now explain how the solution can be reconstructed in the full order space. This reconstruction is simplified with respect to the original version of ALP. This is possible because in ALP-EI we make use of an intermediate space whose basis is the initial basis of size  $N_P$ . Whatever the evolution of the  $N_M$  modes is, it can be described exactly in this extended initial basis, which is in a bijection with the collocation basis on the  $N_P$  points.

PROPOSITION 2.2. *The coordinates  $c(t) \in \mathbb{R}^{N_P}$  of  $\hat{U}(t)$  on the basis  $(\Psi_i)_{i=1\dots N_P}$  are given by*

$$(2.24) \quad c(t) = \Psi^T G \hat{\Phi}(t) \hat{\beta}(t).$$

*Proof.* The basis  $(\Psi_i)_{i=1\dots N_P}$  being orthonormal for the scalar product induced by  $G$ , we have:

$$\hat{\Phi}_i(t) = \sum_{j=1}^{N_P} \langle \Psi_j, \hat{\Phi}_i(t) \rangle_G \Psi_j.$$

Thus:

$$\hat{U}(t) = \sum_{i=1}^{N_M} \hat{\beta}_i(t) \left( \sum_{j=1}^{N_P} \langle \Psi_j, \hat{\Phi}_i(t) \rangle_G \Psi_j \right) = \sum_{i=1}^{N_P} \left( \sum_{j=1}^{N_M} \langle \Psi_i, \hat{\Phi}_j(t) \rangle_G \hat{\beta}_j(t) \right) \Psi_i,$$

thus,  $c_i = \sum_{j=1}^{N_M} \langle \Psi_i, \hat{\Phi}_j(t) \rangle_G \hat{\beta}_j(t)$ . Hence the result since  $\langle \Psi_i, \hat{\Phi}_j(t) \rangle_G$  is the entry  $(i, j)$

of the matrix  $\Psi^T G \hat{\Phi}(t)$ .  $\square$

Following the same approach as in DEIM [3], the solution in the full order space is obtained by keeping the same coordinates  $c(t)$  in the basis  $(\Phi_k(0))_{k=1\dots N_M}$ , i.e.  $u(t) \simeq \Phi(0)c(t)$ . Thus:

$$u(t) \simeq \Phi(0) \Psi^T G \hat{\Phi}(t) \hat{\beta}(t).$$

Defining the  $\mathcal{N} \times N_M$  matrix  $\Pi = \Phi(0) \Psi^T G$ , the reconstruction in the full order space of the reduced solution  $\hat{U}(t)$  is given by:

$$(2.25) \quad u(t) \simeq \Pi \hat{U}(t)$$

Note that  $\Pi$  can be computed off-line once for all. The online cost of the reconstruction is therefore  $\mathcal{N} \times N_P$ .

**2.6. Choice of the interpolation points.** We explain in this section the algorithm used to select the interpolation points. The set of the  $\mathcal{N}$  vertices of the finite element mesh is denoted by  $\Omega_p$ . Consider the set of  $N_P$  eigenmodes, which are represented by the columns of the matrix  $\Phi(0)$ . The index of the first point is chosen such that  $p_1 = \arg \max_{1 \leq i \leq \mathcal{N}} \Phi_{i1}(0)$ . The objective is to define a greedy algorithm to select  $N_P$  points out of  $\mathcal{N}$ . Given a set of indices of points  $\mathcal{P} = \{p_1, \dots, p_n\}$  the index of the  $(n+1)$ -th point will be chosen in  $\Omega_p \setminus \mathcal{P}$ .

When  $n$  points are known, with  $n < N_p$ , the matrix  $\Psi^{(n)} \in \mathbb{R}^{n \times n}$ , whose entries are defined by  $\Psi_{ij}^{(n)} := \Phi_{p_{ij}}(0)$ , is the matrix whose  $j$ -th column is the set of the values of the  $j$ -th eigenfunction evaluated at the  $n$  points whose indices are in  $\mathcal{P}$ . Assume that the matrix  $\Psi^{(n)}$  is full rank, *i.e.*  $\text{rank}(\Psi^{(n)}) = n$ . Define an augmented matrix  $\tilde{\Psi}^{(n)} \in \mathbb{R}^{n \times n+1}$  by appending a column with the values of the  $(n+1)$ -th eigenfunction evaluated at the  $n$  points with indices in  $\mathcal{P}$ :  $\tilde{\Psi}^{(n)} \in \mathbb{R}^{n \times n+1} = [\Psi^{(n)}, \Psi_{p_1 \dots p_n, n+1}]$ , where  $\Psi_{p_1 \dots p_n, n+1}$  is a notation for the components  $p_1, \dots, p_n$  of the vector  $\Psi_{n+1}$ . The rank of the augmented matrix  $\tilde{\Psi}^{(n)}$  is still  $n$ . The objective is to select a point of index  $p_{n+1} \in \Omega_p \setminus \mathcal{P}$  in such a way that the vector  $w := \Psi_{p_{n+1}, 1:n+1} \in \mathbb{R}^{1 \times n+1}$  is “as orthogonal as possible” to the first  $n$  rows of  $\tilde{\Psi}^{(n)}$ . More formally, denoting by  $w_j$  the vector  $\Psi_{p_j, 1:n+1}$ , *i.e.* the values of the  $n+1$  eigenfunctions evaluated in the candidate point  $p_j$ . For every candidate point  $p_j$ , the best least squares approximation of  $w_j$  in terms of the rows of the matrix  $\tilde{\Psi}^{(n)}$  is computed. The point  $p_{n+1}$  is the one for which the approximation is the worst. In other words:

$$p_{n+1} = \arg \max_{p_j \in \Omega_p \setminus \mathcal{P}} \|w_j - \sum_{i=1}^n \alpha_i(w_j) \tilde{\Psi}_{i, 1:n+1}^{(n)}\|_2^2,$$

with

$$\alpha(w_j) = \arg \min_{\alpha \in \mathbb{R}^n} \|w_j - \sum_{i=1}^n \alpha_i \tilde{\Psi}_{i, 1:n+1}^{(n)}\|_2^2.$$

Note that,  $\tilde{\Psi}^{(n)}$  being of rank  $n$ , the matrix  $\tilde{\Psi}^{(n)}(\tilde{\Psi}^{(n)})^T \in \mathbb{R}^{n \times n}$  is symmetric positive definite. The normal equation associated with the least squares approximation of  $w_j$  is therefore well posed.

To conclude, note that necessarily  $\|w_j - \sum_{i=1}^n \alpha_i(w_j) \tilde{\Psi}_{i, 1:n+1}^{(n)}\|_2^2 > 0$  for at least one  $j$ , otherwise this would contradict the fact that the eigenmodes are linearly independent. Thus the rank of the matrix  $\Psi^{(n+1)} \in \mathbb{R}^{n+1 \times n+1}$  is  $n+1$ , so that the hypothesis of full rank of this matrix at the subsequent iteration will be fulfilled. A pseudo-code of the method is presented in Algorithm 1. In Figure 2.2 we show an example of 50 points obtained for the Laplace operator modes on the mesh of a 2D square.

**2.7. Error analysis: Lebesgue constant.** In order to assess the interpolation error associated with the choice of the collocation points for the basis of the Schrödinger eigenfunctions, the Lebesgue constant (see [5, 11]) is investigated as a function of the number of collocation points. The analysis is performed in the spirit of the one proposed in [8] in the context of Reduced Basis methods. The Lebesgue constant is defined by:

$$(2.26) \quad \Lambda_{N_P} = \sup_{x \in \Omega} \sum_{m=1}^{N_P} |V_m^{N_P}(x)|,$$

where the  $V_m^{N_P}(x) \in \mathbb{R}^M$  are characteristic functions satisfying  $V_m^{N_P}(x_{p_n}) = \delta_{mn}$ ,  $1 \leq n, m \leq N_P$ . Let the interpolation error be denoted by  $\epsilon_{N_P}(t)$  and the best approximation error by  $\epsilon_{N_P}^*(t)$ . It can be shown as in [8] that they satisfy  $\epsilon_{N_P}(t) \leq \epsilon_{N_P}^*(t)(1 + \Lambda_{N_P})$ ,  $\forall t \geq 0$ . It is therefore useful to have an idea of the behavior of the Lebesgue constant with respect to the number of collocation points to have an estimation of the interpolation error.

**Algorithm 1** Choice of the interpolation points

---

Let  $p_1 \in \Omega_p$  and  $\Psi^{(1)} = [\Phi_{p_1,1}]$   
**for**  $k = 1 : N_P - 1$  **do**  
 $\mathcal{J}^* = 0.$   
 $p_{k+1} = 0.$   
**for**  $j = 1 : \mathcal{N} - k$  **do**  
 $w_j = [\Phi_{p_j,1} \cdots \Phi_{p_j,k+1}] \in \mathbb{R}^{k+1}$   
 $\alpha^* = \arg \min_{\alpha} \|w_j - \sum_{i=1}^k \alpha_i \tilde{\Psi}_{i,1:k+1}\|_2^2$   
 $\mathcal{J} = \|w_j - \sum_{i=1}^k \alpha_i^* \tilde{\Psi}_{i,1:k+1}\|_2^2$   
**if**  $\mathcal{J} > \mathcal{J}^*$  **then**  
 $\mathcal{J}^* = \mathcal{J}$   
 $p_{k+1} = p_j$   
**end if**  
**end for**  
 $\Psi^{(k+1)} \in \mathbb{R}^{k+1,k+1} = \Phi_{p_1 \dots p_{k+1}, 1:k+1}.$   
**end for**  
**return**  $(p_1, \dots, p_{N_P}), \Psi \in \mathbb{R}^{N_P \times N_P}$

---

$$\left( \begin{array}{c|c} \Psi^{(k)} & \begin{array}{c} \Phi_{p_1,k+1} \\ \vdots \\ \Phi_{p_k,k+1} \end{array} \\ \hline \Phi_{p_{k+1},1} \cdots \Phi_{p_{k+1},k+1} & \end{array} \right)$$

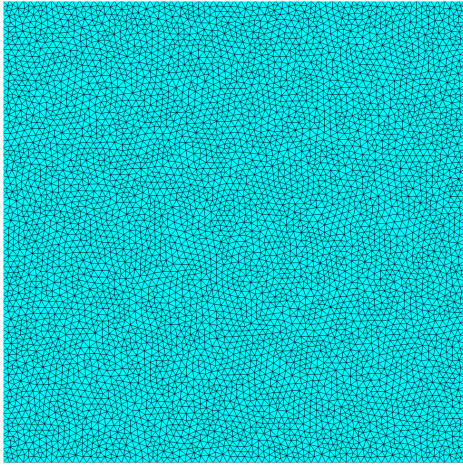
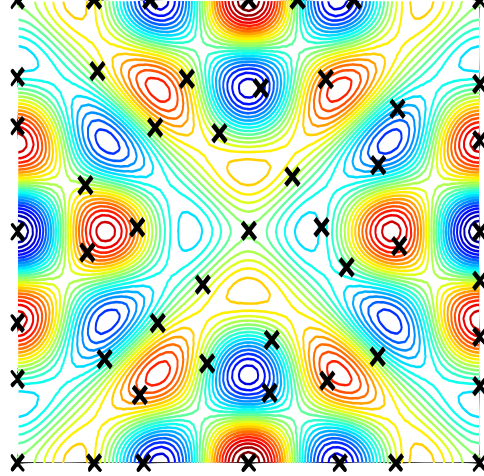
Mesh ( $\mathcal{N} = 5872$ )Collocation points ( $N_p = 50$ )

FIG. 2.2. On the left a FE mesh, on the right the 50th Laplace mode (discretized on the FE mesh) and the correspondig 50 points found with Algorithm 1.

In our procedure for the selection of the points, the values of the Lebesgue constant can be computed straightforwardly. The expansions of  $V_m^{N_P}$  on the finite element basis  $(v_j)_{j=1 \dots \mathcal{N}}$  and on the eigenmodes  $(\varphi_j(x,0))_{1 \dots N_P}$  at  $t = 0$  read

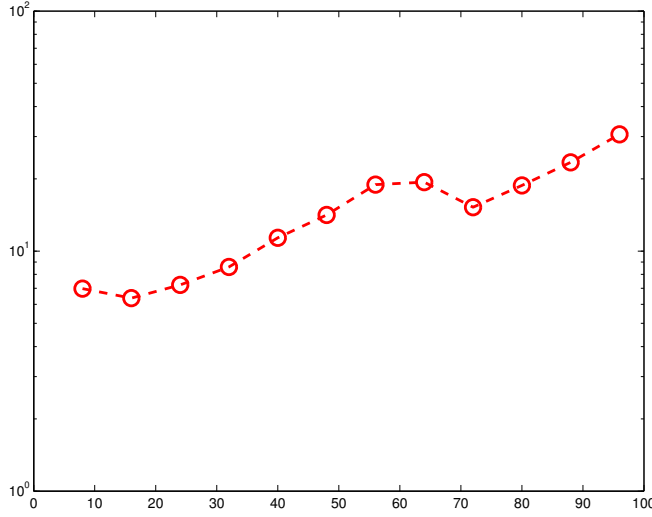


FIG. 2.3. Lebesgue constant  $\Lambda_{N_P}$  as a function of  $N_P$ .

$$V_m^{N_P}(x) = \sum_{j=1}^{\mathcal{N}} V_{jm} v_j(x) = \sum_{j=1}^{N_P} W_{jm} \varphi_j(x, 0) = \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{N_P} \Phi_{ji}(0) W_{im} v_j(x),$$

thus  $\mathbf{V}^{N_P} = \mathbf{\Phi}(0)\mathbf{W}$ , where  $\mathbf{V}^{N_P} = [V_{ij}] \in \mathbb{R}^{\mathcal{N} \times N_P}$  and  $\mathbf{W} = [W_{ij}] \in \mathbb{R}^{N_P \times N_P}$ . By noticing that

$$V_m^{N_P}(x_{p_n}) = \delta_{mn} = \sum_{j=1}^{N_P} W_{jm} \varphi_j(x_{p_n}, 0) = \sum_{j=1}^{N_P} W_{jm} \Psi_{nj},$$

we deduce that  $\mathbf{W} = \mathbf{\Psi}^{-1}$ . Thus:

$$\mathbf{V}^{N_P} = \mathbf{\Phi}(0)\mathbf{\Psi}^{-1}.$$

With Definition (2.26), it is therefore straightforward to deduce  $\Lambda_{N_P}$ . In Figure 2.3 we show the value of the Lebesgue constant varying the number of points. While theoretically it is difficult to obtain estimates which are sharper than a behavior in  $2^{N_P}$ , we can see numerically that the Lebesgue constant grows approximately in a linear way.

**3. Numerical results.** In this section some numerical experiments are presented, on nonlinear reaction diffusion equations. All the test-cases presented are in 2D.

The first test case deals with the reduced integration of the Fisher-Kolmogorov-Petrovski-Piskunov equation (FKPP), for which the nonlinearity is polynomial. Then, several examples of monodomain equations used in electro-physiology are shown, for which the nonlinearity is non-polynomial.

**3.1. FKPP.** The FKPP equation reads:

$$(3.1) \quad \begin{cases} \frac{\partial u}{\partial t} - \Delta u = cu(1-u), & \Omega = [0, 1]^2, \\ u = 0, & \partial\Omega. \end{cases}$$

The ALP-EI scheme is detailed for this equation, to provide a less abstract example of the discretisation. The solution  $u$  is approximated on the first  $N_M$  modes:

$$(3.2) \quad \sum_{i=1}^{N_M} \partial_t \beta_i \varphi_i + \beta_i \partial_t \varphi_i - \beta_i \Delta \varphi_i = cu(1-u).$$

The spectral problem is substituted:

$$(3.3) \quad -\Delta \varphi_i = \chi u \varphi_i + \lambda_i \varphi_i \Rightarrow \sum_{i=1}^{N_M} \partial_t \beta_i \varphi_i + \beta_i \partial_t \varphi_i + \beta_i (\chi u \varphi_i + \lambda_i \varphi_i) = cu(1-u).$$

After some algebra and by noticing that  $\sum_i \beta_i u \varphi_i = u^2$ , the expression becomes:

$$(3.4) \quad \sum_{i=1}^{N_M} \partial_t \beta_i \varphi_i + \beta_i \partial_t \varphi_i = cu(1-u) - \chi u^2 - \sum_{i=1}^{N_M} \beta_i \lambda_i \varphi_i.$$

This equation is discretised on the  $N_P$  points and the equations for the coefficients  $\hat{\beta}$  is found by projecting the equation on the basis:

$$(3.5) \quad \partial_t \hat{\beta} + \hat{M} \hat{\beta} = (cI + \hat{\Lambda}) \hat{\beta} - (c + \chi) \langle \hat{u}^2, \hat{\Phi} \rangle.$$

Remark that this equation does not contain the discretisation of space differential operators, by virtue of the substitution of the spectral problem. The equation has been discretised by a mixed semi-implicit scheme of the form :

$$(3.6) \quad \left( \frac{I}{\Delta t} - \frac{c + \hat{\Lambda}^{(n)}}{2} \right) \hat{\beta}^{(n+1)} = \left( \frac{I}{\Delta t} + \frac{c + \hat{\Lambda}^{(n)}}{2} \right) \hat{\beta}^{(n)} - \hat{M}^{(n)} \hat{\beta}^{(n)} - (c + \chi) \langle \hat{u}^{(n)2}, \hat{\Phi} \rangle$$

The full-order problem is defined on the unitary square  $\Omega = [0, 1]^2$ , discretised by a  $P_1$  finite element, the number of degrees of freedom is  $\mathcal{N} \approx 5 \cdot 10^3$ . The initial solution is  $u_0 = g(\mu, \sigma^2)$  where  $g$  is a gaussian centered around  $\mu = [0.25, 0.25]$  and  $\sigma^2 = \text{diag}[0.01, 0.01]$ .

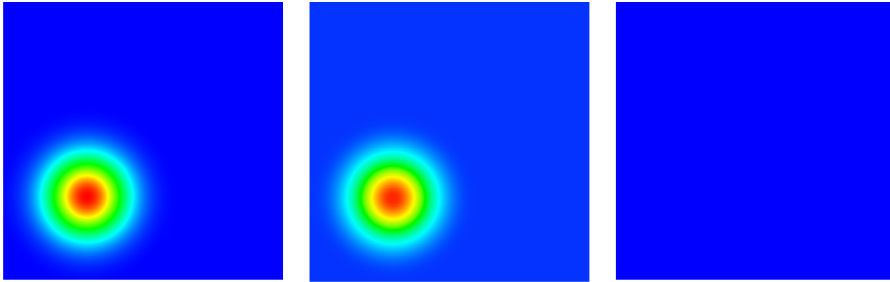
Several test-cases were performed in order to assess the properties of the method. The results are shown in Table 3.1, when the number of points  $N_P$  and the number of modes  $N_M$  is varied. As expected, the results show a monotonic behavior. At fixed number of modes, the error decreases when the number of collocation points are increased, and the speed-up decreases. Similarly, by keeping fix the number of points, the error decreases when the number of modes are increased, and the speed-up decreases. Remark that the speed-up obtained is significant, being of about two orders of magnitude.

In Figure 3.1 we compare the FE solution (left) with the ALP-EI method for  $N_m = 15$ ,  $N_p = 50$  (middle) and we show the relative error (right)

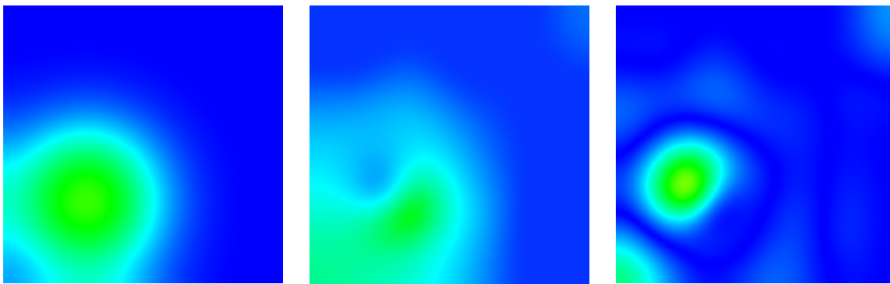
$$(3.7) \quad \text{error}(t^n) = \frac{|v_m(t^n) - \hat{\Phi}(t^n) \beta(t^n)|}{\max |v_m(t^n)|}$$

for different time-steps. We see that the results are satisfactory with a very low number of modes and interpolation points.

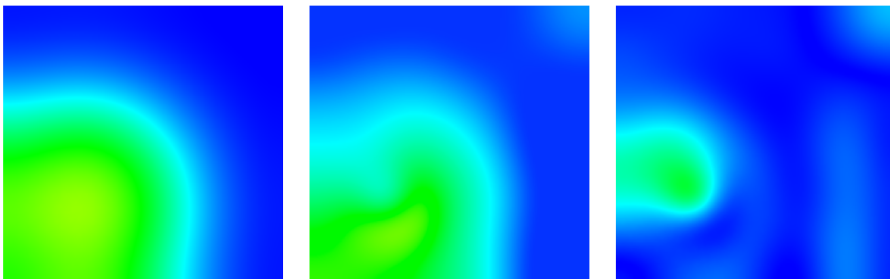
Time = 0 ms



Time = 0.1 ms



Time = 0.2 ms



Time = 0.3 ms

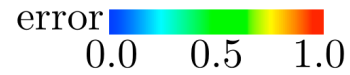
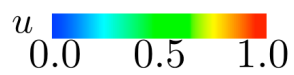
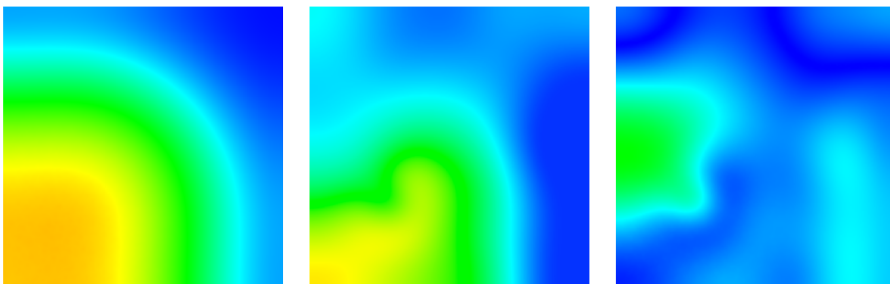


FIG. 3.1. 2D test case for problem (3.1). FEM solution (left), ALP-EI solution with  $N_m = 15$ ,  $N_p = 50$  (middle) and relative error (right).

$N_M$	$N_P$	$\ e\ _{L^2(L^2)}$	time per iter. (msec)	speed-up
25	101	$1.81 \times 10^{-2}$	1.3674	184
	150	$1.69 \times 10^{-2}$	3.1339	80
	200	$1.27 \times 10^{-2}$	6.2504	40
30	101	$1.68 \times 10^{-2}$	1.7445	144
	150	$1.67 \times 10^{-2}$	3.8966	64
	200	$1.24 \times 10^{-2}$	7.4561	34
35	101	$1.50 \times 10^{-2}$	2.1159	119
	150	$1.48 \times 10^{-2}$	4.7405	53
	200	$1.12 \times 10^{-2}$	9.0164	28
40	101	$1.48 \times 10^{-2}$	2.5028	100
	150	$1.44 \times 10^{-2}$	5.6005	45
	200	$1.10 \times 10^{-2}$	10.7833	23

TABLE 3.1

Relative error in  $l^2(L^2)$  norm, time per iteration and speed-up compared to FEM (5k dof, time per iteration = 251.3866 msec) varying number of modes (from 25 to 50) and number of points (from 101 to 200) for FKPP equation.

**3.2. Cardiac electrophysiology.** We are now interested in applying the ALP-EI method to some non-polynomial nonlinear test cases. Let us concentrate on the so-called *monodomain* equations [4] used to describe the electrical potential in a cardiac tissue. Monodomain equations are a simplified version of the *bidomain* equations [14]. Even if in some cases, such as for electrocardiogram or defibrillation simulation [2], bidomain equations are needed, in many cases monodomain equations prove to be sufficient [4].

In their general formulation, monodomain equations read

$$(3.8) \quad \begin{cases} A_m \left( C_m \frac{\partial v_m}{\partial t} + I_{\text{ion}}(v_m, w) \right) - \text{div}(\sigma_i \nabla v_m) = A_m I_{\text{app}}(x, t), \\ \frac{\partial w}{\partial t} - g(v_m, w) = 0, \end{cases}$$

with the following boundary conditions on  $\partial\Omega$

$$(3.9) \quad \{ \sigma_i \nabla v_m \cdot \mathbf{n} = 0, \}$$

where  $v_m$  represents the transmembrane potential,  $A_m$  and  $C_m$  are the ratio of membrane area per unit volume and the membrane capacitance per area respectively,  $\sigma_i$  denotes the intra-cellular conductivity tensor (see for instance [12]) and  $I_{\text{app}}$  is a given source term. The nonlinear reaction term  $I_{\text{ion}}(v_m, w)$  representing a ionic current is given by the solution of an ODE system. In what follows we consider the Mitchell and Schaeffer ionic model [10]

$$(3.10) \quad \begin{aligned} I_{\text{ion}}(v_m, w) &= w \frac{v_m^2(1-v_m)}{\tau_{\text{in}}} + \frac{v_m}{\tau_{\text{out}}}, \\ g(v_m, w) &= \begin{cases} \frac{w-1}{\tau_{\text{open}}}, & v_m < v_{\text{gate}}, \\ \frac{w}{\tau_{\text{close}}}, & v_m > v_{\text{gate}}, \end{cases} \end{aligned}$$

where  $\tau_{\text{in}}$ ,  $\tau_{\text{out}}$ ,  $\tau_{\text{open}}$ ,  $\tau_{\text{close}}$ ,  $v_{\text{gate}}$  are scalar parameters.

In order to apply the ALP-EI method, we follow the same steps given in the previous example. To take into account anisotropic  $\sigma_i$  due to the presence of fibers in the cardiac tissue, we define the spectral operator used to compute the initial basis as

$$(3.11) \quad \mathcal{L}(u)\varphi = -\text{div}(\sigma_i \nabla \varphi) - \chi u \varphi,$$

where the solution  $u$  is the transmembrane potential  $v_m$ .

Then we approximate the transmembrane potential  $v_m$  by  $v_m \simeq \sum \beta_i \varphi_i$ , and consider problem (3.8) approximated on the first  $N_M$  modes:

$$(3.12) \quad A_m C_m \sum_{i=1}^{N_M} \partial_t \beta_i \varphi_i + \beta_i \partial_t \varphi_i - \sum_{i=1}^{N_M} \beta_i \text{div}(\sigma_i \nabla \varphi_i) = -A_m (I_{\text{ion}}(v_m, w) - I_{\text{app}})$$

Using  $-\text{div}(\sigma_i \nabla \varphi_i) \varphi_i = \chi v_m \varphi_i + \lambda_i \varphi_i$  in this relation:

$$(3.13) \quad A_m C_m \sum_{i=1}^{N_M} \partial_t \beta_i \varphi_i + \beta_i \partial_t \varphi_i - \sum_{i=1}^{N_M} \beta_i (\chi v_m \varphi_i + \lambda_i \varphi_i) = -A_m (I_{\text{ion}}(v_m, w) - I_{\text{app}}).$$

After some algebra and by noticing that  $\sum_i \beta_i v_m \varphi_i = v_m^2$ , the expression becomes:

$$(3.14) \quad A_m C_m \sum_{i=1}^{N_M} \partial_t \beta_i \varphi_i + \beta_i \partial_t \varphi_i = -A_m (I_{\text{ion}}(v_m, w) - I_{\text{app}}) - \chi v_m^2 - \sum_{i=1}^{N_M} \beta_i \lambda_i \varphi_i.$$

This equation is discretised on the  $N_P$  points and the equations for the coefficients  $\hat{\beta}$  is found by projecting the equation on the basis:

$$(3.15) \quad A_m C_m (\partial_t \hat{\beta} + M \hat{\beta}) = -A_m \langle (I_{\text{ion}}(\hat{v}_m, \hat{w}) - I_{\text{app}}), \hat{\Phi} \rangle + -\chi \langle \hat{v}_m^2, \hat{\Phi} \rangle + \Lambda \hat{\beta}.$$

Remark that the nonlinear ODE system (3.10) is solved point-wise on the  $N_p$  points.

The full-order problem is defined on  $\Omega = [0, 1]^2$ , discretised by a  $P_1$  finite element, the number of degrees of freedom is  $\mathcal{N} \approx 5 \cdot 10^3$ , a second order Backward Difference method is applied for the time discretization. Both full-order and reduced-order problems are discretized with a time step  $\delta t = 0.01\text{ms}$ . Parameters are taken as in Table 3.2.

First, we consider an homogeneous cardiac tissue on a 2D domain where a source term not included in the initial basis is introduced. Then, a spatial heterogeneity is introduced: the parameter that regulates the depolarization plateau duration is changed as in the cardiac tissue. It should be noted that with reduced-order methods like POD, this kind of test cases is difficult to handle without considering a huge amount of scenarios in the offline stage.

$A_m$	$C_m$	$\sigma_i$	$\tau_{\text{in}}$	$\tau_{\text{out}}$	$\tau_{\text{open}}$	$\tau_{\text{close}}$	$v_{\text{gate}}$
2000.0	0.1	1.0	4.0	50.0	100.0	80.0	0.13

TABLE 3.2

*Bidomain equations and Mitchell and Schaeffer ionic model parameters.*



**Source terms.** First, we consider the monodomain equations with the Mitchell and Schaeffer model, without fiber tensors orientation and with homogeneous parameters. The challenging point is the treatment of the non-polynomial term in the Mitchell and Schaeffer ionic model.

The initial basis is computed using the FE solution at time  $t = 5\text{ms}$ , with  $\chi = 25$ , and the solution is run with  $N_M = 25$  basis modes. In Figure 3.2 the results with the ALP-EI method (middle) are compared to the FE ones (left). We can see that the reduced order solution is very close to the FE element solution. This can also be observed in the relative error in Figure 3.2 right. The error is less than 10% for most of the time except at about 25ms when the propagation front “exits” the domain, but in all cases it does not exceed 30%.

Then, a source term located in a different position compared to the first one is applied. After the end of the complete cardiac cycle and whole repolarization of the tissue, the second applied stimulus is located in the top-left corner of the domain as shown in Figure 3.3 (first row). The application of a new source term is particularly simple in the framework of the ALP-EI algorithm.

The results in Figure 3.3 show a good agreement between the FE and the reduced-order solutions, which is run with  $\chi = 25$  and  $N_M = 25$  modes. The error presents some oscillations at the moment of the source term application, probably due to the change of direction of the first modes of the basis, but it is in general of very low values, at most less than 10%.

Several tests are run with different number of modes  $N_m$  and of points  $N_p$ . Results are schematized in Table 3.3. We can observe that satisfactory results both in term of relative error, which is limited to  $10^{-2}$  for small values of  $N_m$  and  $N_p$ , and of speed-up of the method.

**Heterogeneous ionic parameters.** We are now interested in introducing some heterogeneities in the ionic parameters. In particular, we reproduce the cardiac tissue heterogeneity by considering three different cell types: endocardial, mid-myocardial and epicardial cells. The parameter  $\tau_{\text{close}}$  of the ionic model varies in these three layers illustrated in Figure 3.4 top-left, and takes values given in Table 3.4. Owing to this heterogeneity, the solution has a repolarization front which propagates in the opposite direction to the depolarization one.

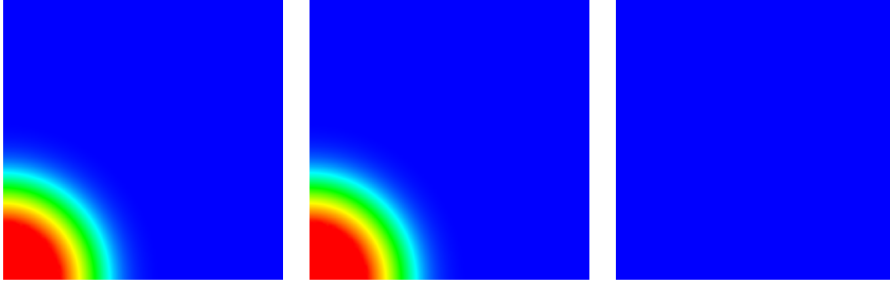
The ROM simulation is run with  $N_M = 25$  modes and  $\chi = 25$ , and the initial basis is computed from the FE solution at time  $t = 5\text{ms}$ . We can see in Figure 3.4 that the reduced-order solution (middle) is very close to the FE one (left) both in the depolarization phase (second row) and in the repolarization one (third row), and the error takes locally values of at most 30% and does not exceed 5% elsewhere.

Also in this case, several tests varying the number of modes  $N_m$  and the number of points  $N_p$  are run. Results of Table 3.5 show satisfactory behavior of the method both in terms of relative error and speed-up of the resolution.

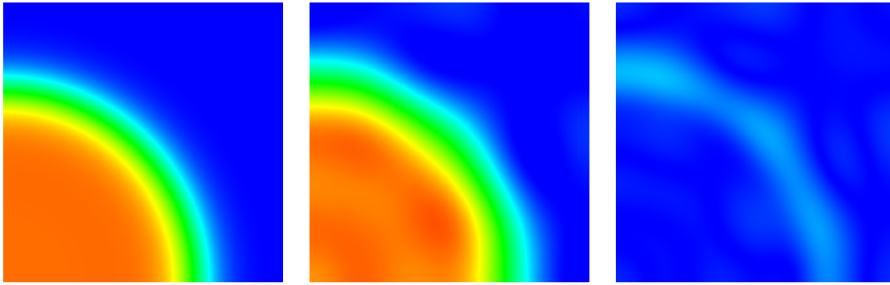
**4. Improved approximation of the eigenmodes evolution.** During our numerical tests, we observed that, in some situations, it may be useful to use an improved approximation of the time evolution of the eigenmodes. In this Section, we present a strategy to do so, and we illustrate it on a simple linear advection equation.

**4.1. Basis dynamics.** The basis time derivative can be approximated as the sum of an endomorphism and a linear transformation defined in the space orthogonal to the space spanned by the modes. In particular, let us define  $R$  the matrix of the

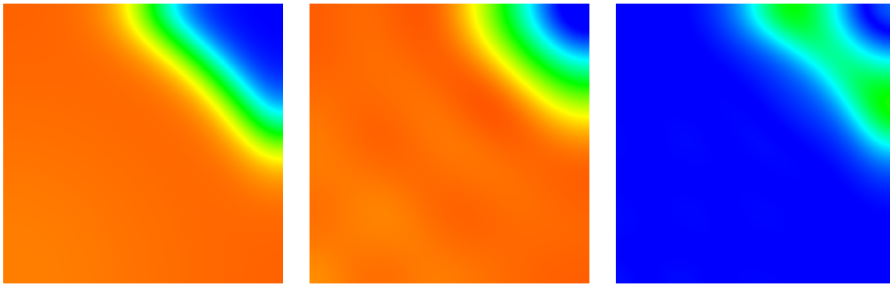
Time = 5 ms



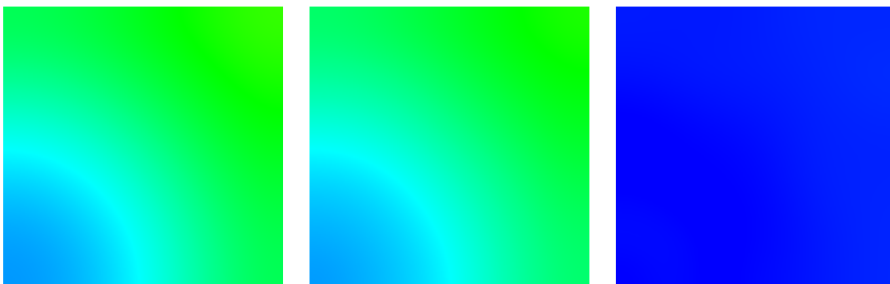
Time = 15 ms



Time = 25 ms



Time = 125 ms

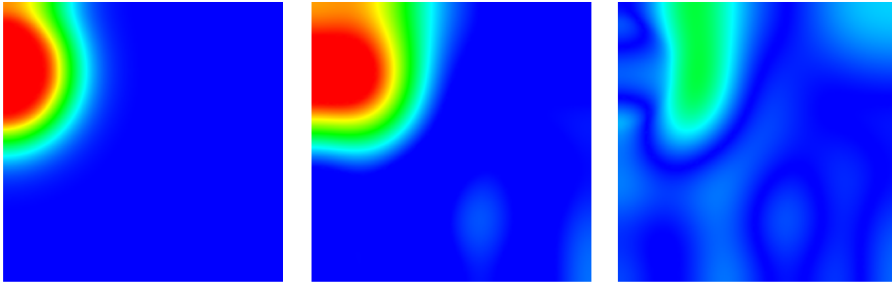


$v_m$  0.0 0.5 1.0

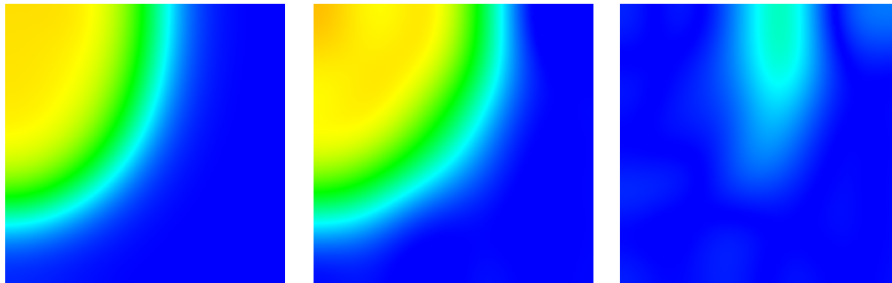
error 0.0 0.5 1.0

FIG. 3.2. 2D test case with homogeneous parameters. FEM solution (left), ALP-EI solution (middle) and relative error (right).

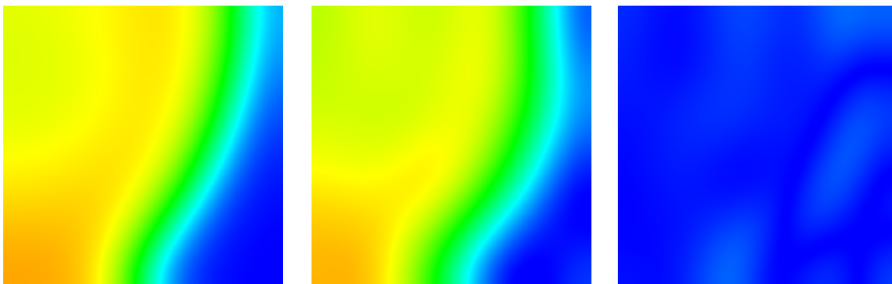
Time = 205 ms



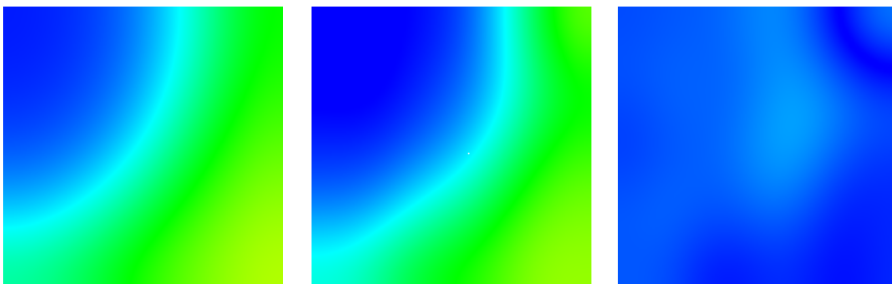
Time = 220 ms



Time = 235 ms



Time = 300 ms



$v_m$  0.0 0.5 1.0

error 0.0 0.5 1.0

FIG. 3.3. 2D test case with source term. FEM solution (left), ALP-EI solution (middle) and relative error (right).

$N_M$	$N_P$	$\ e\ _{l^2(l^2)}$	time per iter. (msec)	speed-up
10	26	$2.52 \times 10^{-2}$	0.0892	330
	30	$2.44 \times 10^{-2}$	0.1050	280
	41	$2.75 \times 10^{-2}$	0.1521	193
	50	$2.83 \times 10^{-2}$	0.1990	147
	62	$3.12 \times 10^{-2}$	0.2723	108
15	26	$1.41 \times 10^{-2}$	0.1583	185
	30	$1.81 \times 10^{-2}$	0.1845	159
	41	$2.28 \times 10^{-2}$	0.2683	109
	50	$2.16 \times 10^{-2}$	0.3454	85
	62	$2.81 \times 10^{-2}$	0.4692	62
21	26	$1.32 \times 10^{-1}$	0.2735	107
	30	$5.28 \times 10^{-2}$	0.3169	92
	41	$1.80 \times 10^{-2}$	0.4515	65
	50	$1.50 \times 10^{-2}$	0.5757	51
	62	$2.47 \times 10^{-2}$	0.7624	38
25	26	$2.20 \times 10^{-1}$	0.3754	78
	41	$2.19 \times 10^{-2}$	0.6050	48
	50	$1.24 \times 10^{-2}$	0.7606	38
	62	$2.39 \times 10^{-2}$	0.9960	29
30	30	$2.14 \times 10^{-1}$	0.5989	49
	41	$1.77 \times 10^{-2}$	0.8244	35
	50	$1.27 \times 10^{-2}$	1.0421	28
	62	$2.39 \times 10^{-2}$	1.3311	22

TABLE 3.3

Relative error in  $l^2(l^2)$  norm, time per iteration and speed-up compared to FEM (5k dof, time per iteration = 29.4410 msec) varying number of modes (from 10 to 30) and number of points (from 26 to 62) for monodomain equation with a source term.

$\tau_{\text{close}}^{\text{endo}}$	$\tau_{\text{close}}^{\text{Mcell}}$	$\tau_{\text{close}}^{\text{epi}}$
90.0	70.0	50.0

TABLE 3.4

Ionic parameters for heart model.

residual in the basis evolution equation:

$$(4.1) \quad \partial_t \Phi = \Phi M + R,$$

where  $R$  is orthogonal to the space spanned by the modes and  $M$  is the representation of  $\mathcal{M}$  on the basis.

In order to practically compute  $R$  in an efficient way, the above identity is specialised for the collocation space of size  $N_P$ , that is in a bijection with the space spanned by  $N_P$  modes at the initial time. An orthogonal basis, *i.e.* a basis of the orthogonal complement to  $\hat{\Phi}$ , is defined as

$$(4.2) \quad \Phi^\perp = [\Psi_{N_M+1} \cdots \Psi_{N_P}] - \hat{\Phi} \hat{\Phi}^T G [\Psi_{N_M+1} \cdots \Psi_{N_P}],$$

where  $\Psi_i$  is the  $i$ -th column of  $\Psi$ . Only few elements of  $\Psi$  are retrieved, let us call the dimension of  $\Phi^\perp$   $N^\perp \leq N_P - N_M$ . The partial derivatives of the modes is

$N_M$	$N_P$	$\ e\ _{l^2(l^2)}$	time per iter. (msec)	speed-up
10	26	$4.55 \times 10^{-2}$	0.0852	374
	30	$4.60 \times 10^{-2}$	0.1022	311
	41	$4.36 \times 10^{-2}$	0.1482	215
	50	$4.41 \times 10^{-2}$	0.1962	162
	62	$4.36 \times 10^{-2}$	0.2699	118
15	26	$4.27 \times 10^{-2}$	0.1541	206
	30	$4.28 \times 10^{-2}$	0.1778	179
	41	$4.21 \times 10^{-2}$	0.2605	122
	50	$4.21 \times 10^{-2}$	0.3360	94
	62	$4.15 \times 10^{-2}$	0.4636	68
21	26	$4.06 \times 10^{-2}$	0.2604	122
	30	$4.32 \times 10^{-2}$	0.3090	103
	41	$4.07 \times 10^{-2}$	0.4338	73
	50	$4.05 \times 10^{-2}$	0.5611	56
	62	$4.02 \times 10^{-2}$	0.7566	42
25	26	$1.08 \times 10^{-2}$	0.3517	90
	30	$1.92 \times 10^{-2}$	0.4078	78
	41	$1.74 \times 10^{-2}$	0.5779	55
	50	$1.30 \times 10^{-2}$	0.7409	43
	62	$1.31 \times 10^{-2}$	0.9928	32
30	30	$3.94 \times 10^{-2}$	0.5657	56
	41	$3.91 \times 10^{-2}$	0.7900	40
	50	$3.94 \times 10^{-2}$	1.0106	31
	62	$3.94 \times 10^{-2}$	1.3259	24

TABLE 3.5

Relative error in  $l^2(l^2)$  norm, time per iteration and speed-up compared to FEM (5k dof, time per iteration = 31.8843 msec) varying number of modes (from 10 to 30) and number of points (from 26 to 62) for monodomain equation with heterogeneous  $\tau_{close}$  parameter.

approximated by

$$(4.3) \quad \partial_t \hat{\Phi} \simeq \hat{\Phi} M + \Phi^\perp C,$$

and this expression is injected into equation (2.12), leading to

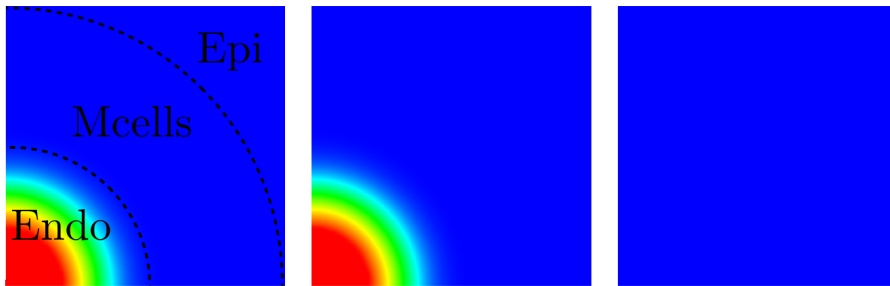
$$(4.4) \quad G \hat{\Phi} \Lambda M + L \Phi^\perp C - G \hat{\Phi} M \Lambda - G \Phi^\perp C \Lambda = G \hat{\Phi} \dot{\Lambda} + \chi G \partial_t \hat{u} \odot \hat{\Phi}.$$

The projection of this equation onto  $\Phi$  has already been computed and leads to the representation of the evolution operator and the time derivative of the eigenvalues, since  $\Phi^\perp$  is by construction orthogonal to  $\Phi$ . The projection onto  $\Phi^\perp$  allows us to determine the expression of  $C$ :

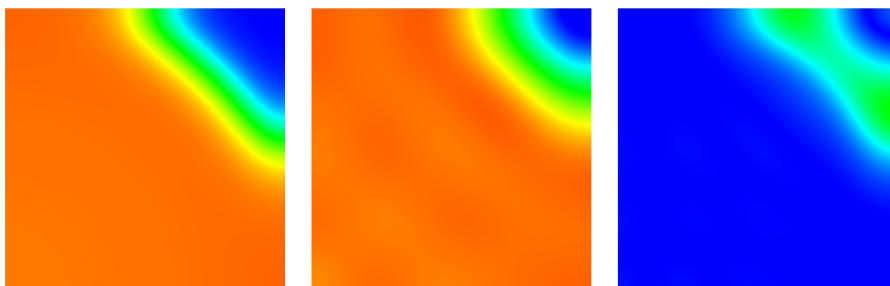
$$(4.5) \quad (\Phi^\perp)^T L \Phi^\perp C - (\Phi^\perp)^T G \Phi^\perp C \Lambda = \chi (\Phi^\perp)^T G \partial_t \hat{u} \odot \hat{\Phi}.$$

Thus, a matrix equation for  $C$  can be written for each mode separately. It can be demonstrated that the system matrix  $(\Phi^\perp)^T L \Phi^\perp - \lambda_i (\Phi^\perp)^T G \Phi^\perp$ ,  $i = 1, \dots, N_M$ , for each mode is positive definite. If  $\partial_t \hat{u} \odot \hat{\Phi}$  has a null projection in the space spanned by  $\Phi^\perp$ ,  $C$  vanishes identically. Otherwise, the derivatives of the modes have a non-vanishing projection onto the orthogonal space if and only if the image of the

Time = 5 ms



Time = 25 ms



Time = 115 ms

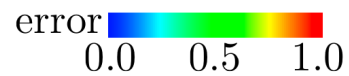
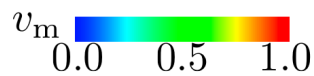
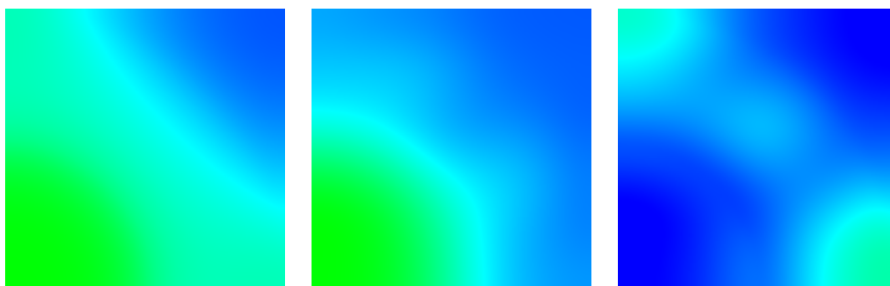


FIG. 3.4. 2D test case with heterogeneous parameter  $\tau_{close}$ . FEM solution (left), ALP-EI solution (middle) and relative error (right).

operator  $\partial_t \hat{u} \odot \hat{\Phi}$  has. This, indeed, can be exploited to setup an *a posteriori* criterion to decide whether it is useful to compute the orthogonal complement part of the time derivative of the modes. The following simple numerical experiment on a linear advection equation provides a paradigmatic example of a situation in which the time derivative has a significant projection in the orthogonal complement of the basis.

**4.2. Application: linear advection equation.** To illustrate the construction explained in the previous section, we consider a linear advection equation in 1D on the

interval  $\Omega = [0, 1]$ . The main difference with respect to the parsimonious discretisation presented so far is that, for the linear advection problem, the operator  $\partial_x$  cannot be substituted by exploiting the spectral problem. For the present case, which provides also an example on how the proposed methodology can be extended to a broader class of problems, we decided to represent the operator  $\partial_x$  on the space spanned by the modes  $\Psi$ . The resulting matrix  $D_x \in \mathbb{R}^{N_P \times N_P}$  is constructed as it is done in the spectral collocation approaches (see [13] for a comprehensive overview):

$$(4.6) \quad D_x \Psi = \mathcal{P}(\partial_x \Phi_0),$$

that is, the application of the matrix  $D_x$  to every collocated mode  $\Psi$  equals the collocation of the derivative performed in the full-order finite element space. This ensures that for every function belonging to the space spanned by  $\Psi$  the derivative has the same accuracy as that obtained in the full-order space.

An ALP-EI discretisation is performed by considering  $N_P = 40$  points and  $N_M = (10, 15, 20)$ ,  $\Delta t = 5 \cdot 10^{-3}$  and a Runge-Kutta implicit mid-point scheme in time. The exact solution is:  $u = \exp(-250(x - 0.6t - 0.2)^2)$  for  $t \in [0, 1]$ . Two sets of experiments are performed, one in which the orthogonal complement part of the derivative is neglected and one in which it is taken into account. The results are

$N_M$	$\Phi^\perp$	$\ e\ _{L^2(L^2)}$
10	no	0.3119
10	yes	0.0472
15	no	0.0851
15	yes	0.0195
20	no	0.0219
20	yes	0.0137

TABLE 4.1

*Relative  $\ell_2(\ell_2)$  error on the evolution of a linear advection equation when  $N_P = 40$ ,  $N_M = (10, 15, 20)$  when the projection onto the orthogonal complement of the basis is considered and when it is neglected.*

reported in Table 4.1. The difference between the results obtained by considering and by neglecting the projection of the derivative of the modes on the orthogonal complement is very significant, especially when the number of modes is low.

## REFERENCES

- [1] M. Barrault, Y. Maday, N. C. Nguyen, and A. T. Patera. An “empirical interpolation” method: Application to efficient reduced-basis discretization of partial differential equations. *C. R. Math. Acad. Sci. Paris*, 339:667–672, 2004.
- [2] M. Boulakia, S. Cazeau, M.A. Fernández, J-F. Gerbeau, and N. Zemzemi. Mathematical modeling of electrocardiograms: a numerical study. *Annals of Biomedical Engineering*, 38(3):1071–1097, 2010.
- [3] S. Chaturantabut and D. Sorensen. Nonlinear model reduction via discrete empirical interpolation. *SIAM Journal of Scientific Computing*, 32(5):2737–2764, 2010.
- [4] P. Colli Franzone, L.F. Pavarino, and B. Taccardi. Simulating patterns of excitation, repolarization and action potential duration with cardiac Bidomain and Monodomain models. *Mathematical Biosciences*, 197(1):35–66, 2005.
- [5] P. Erdős. Problems and results on the theory of interpolation, II. *Acta Math. Acad. Sci.*, 12:235–244, 1961.
- [6] J-F. Gerbeau and D. Lombardi. Approximated Lax Pairs for the Reduced Order Integration of Nonlinear Evolution Equations. *Journal of Computational Physics*, 265:246–269, 2014.
- [7] J-F. Gerbeau, D. Lombardi, and E. Schenone. Reduced order model in cardiac electrophysiology with approximated Lax pairs. *Advances in Computational Mathematics*, 41(5):1103–1130, 2015.
- [8] M. A. Grepl, Y. Maday, N. C. Nguyen, and A. T. Patera. Efficient reduced-basis treatment of nonaffine and nonlinear partial differential equation. *ESAIM: Mathematical Modelling and Numerical Analysis*, 41(3):575–605, 2007.
- [9] P. D. Lax. Integrals of nonlinear equations of evolution and solitary waves. *Comm. Pure Appl. Math.*, 21:467–490, 1968.
- [10] C.C. Mitchell and D.G. Schaeffer. A two-current model for the dynamics of cardiac membrane. *Bulletin Math. Bio.*, 65:767–793, 2003.
- [11] T. J. Rivlin. *An introduction to the approximation of functions*. Dover Publications Inc., New York, 1981.
- [12] D.D. Streeter. Gross morphology and fiber geometry of the heart. *Handbook Physiology, The cardiovascular system*, 1:61–112, 1979.
- [13] Lloyd N Trefethen. *Spectral methods in MATLAB*, volume 10. Siam, 2000.
- [14] L. Tung. *A bi-domain model for describing ischemic myocardial d-c potentials*. PhD thesis, Massachusetts Institute of Technology. Dept. of Electrical Engineering and Computer Science, 1978.