Convergence analysis of BDDC preconditioners for composite DG discretizations of the cardiac cell-by-cell model

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Joint work with

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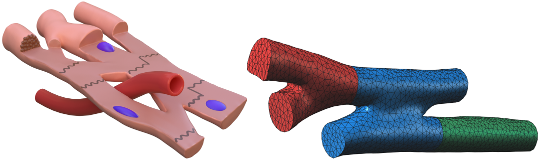

Microcard workshop 2023
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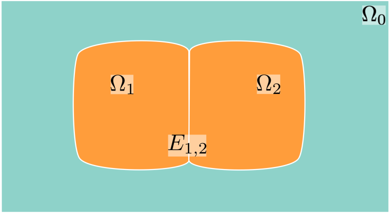
Step 1: multi-cells EMI model

$$\begin{cases} -\operatorname{div}(\sigma_e \nabla u_e) = 0 & \text{in } \Omega_e = \Omega_0 \\ -\operatorname{div}(\sigma_i \nabla u_i) = 0 & \text{in } \Omega_i, \quad i = 1, \ldots, N \\ -n_i^T \sigma_i \nabla u_i = C_m \dfrac{\partial v_{ij}}{\partial t} + F(v_{ij}) & \text{on } E_{1,2} = \overline{\Omega}_i \cap \overline{\Omega}_j \subset \partial \Omega_i \end{cases}$$

$+$ ionic model

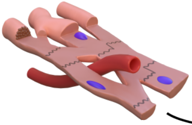
- $v_{ij} = u_i - u_j$ represents the jump in the value of the electric potentials between cells i and j
- $F(v_{ij})$:

$$F(v_{ij}) = \begin{cases} I_{\text{ion}}(v_{ij}, c, w) \\ G(v_{ij}) \end{cases}$$



Extracellular space – cell **M**embrane – **I**ntracellular space.
A Tveito, K-A Mardal, ME Rognes. *Modeling Excitable Tissue – The EMI Framework* (2021).

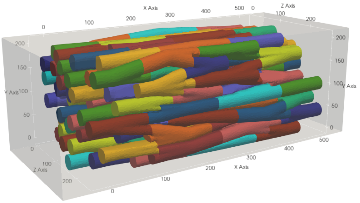
Step 2:

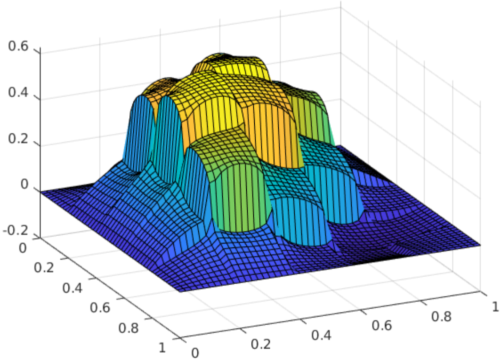


$$K\mathbf{u} = \mathbf{f}$$

?

Microscopic model   Algebraic system   Suitable solver?





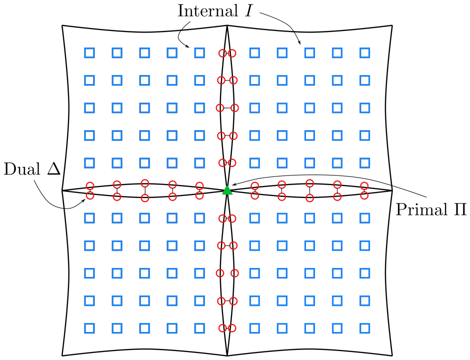
Idea

Solve iteratively, starting from an initial guess and building an algorithm that converges to the unknown solution by solving local problems.

From $K\mathbf{u} = \mathbf{f}$ on Ω, we solve local problems $K^{(i)}\mathbf{u}^{(\mathbf{i})} = \mathbf{f}^{(\mathbf{i})}$ on each subdomain Ω_i, where

$$K^{(i)} = \begin{bmatrix} K_{II}^{(i)} & K_{I\Delta}^{(i)} & K_{I\Pi}^{(i)} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} & K_{\Pi\Pi}^{(i)} \\ K_{\Pi I}^{(i)} & K_{\Pi\Delta}^{(i)} & K_{\Pi\Pi}^{(i)} \end{bmatrix},$$

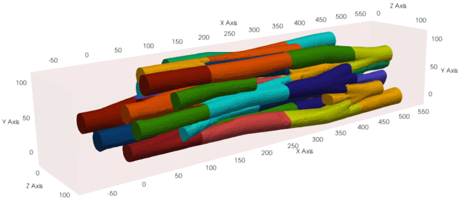
$$\mathbf{u}^{(\mathbf{i})} = \begin{bmatrix} \mathbf{u}_{\mathbf{I}}^{(\mathbf{i})} \\ \mathbf{u}_{\boldsymbol{\Delta}}^{(\mathbf{i})} \\ \mathbf{u}_{\boldsymbol{\Pi}}^{(\mathbf{i})} \end{bmatrix}, \qquad \mathbf{f}^{(\mathbf{i})} = \begin{bmatrix} \mathbf{f}_{\mathbf{I}}^{(\mathbf{i})} \\ \mathbf{f}_{\boldsymbol{\Delta}}^{(\mathbf{i})} \\ \mathbf{f}_{\boldsymbol{\Pi}}^{(\mathbf{i})} \end{bmatrix}.$$

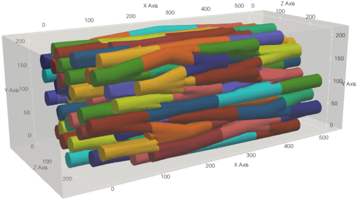


Idea

Solve iteratively, starting from an initial guess and building an algorithm that converges to the unknown solution by solving local problems.

What if we have problems with discontinuities ALONG the interfaces?
How can we deal with such methods?





Courtesy of Dr. M. Potse (IHU LIRYC & Inria Bordeaux Sud-Ouest)

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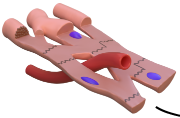
Can we design a preconditioner such that

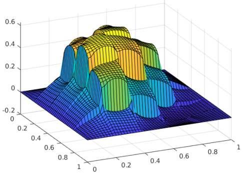
- ◇ the dual-primal algorithm is not modified
- ◇ and natural discontinuities are preserved?



Microscopic model

$$K\mathbf{u} = \mathbf{f}$$

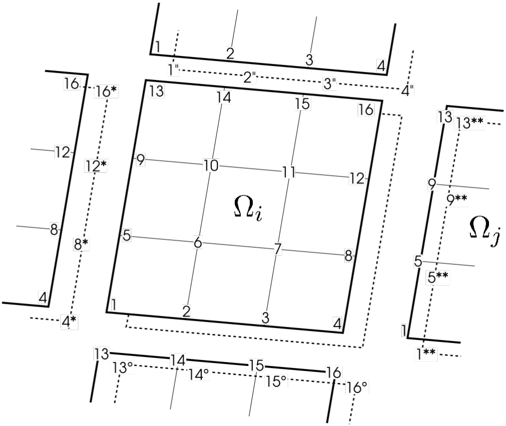
Algebraic system

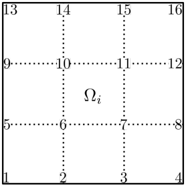


Model-based
Domain Decomposition solver

Extended dual and primal spaces

Necessity of enriching dual and primal spaces by adding constraints through the domains





- can pass information between domains
- do not influence discontinuity of global solution

Decomposition of the solution

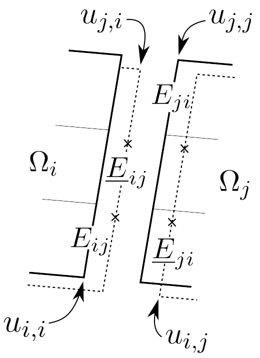
- "Fat" space: $\Omega_i' = \overline{\Omega}_i \cup \bigcup_{j \in \mathcal{E}_i^0} \underline{E}_{ji}$
- Associated local FE space:

$$W_i(\Omega_i') = V_i(\overline{\Omega}_i) \times \prod_{j \in \mathcal{E}_i^0} W_i(\underline{E}_{ji})$$

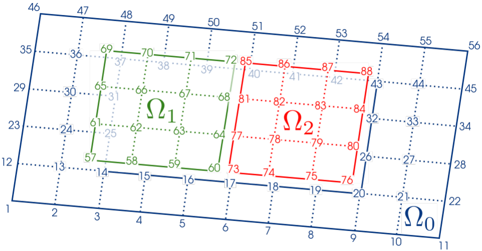
- "Fat" interface subspace: $\Gamma_i' := \Gamma_i \cup \left\{ \bigcup_{j \in \mathcal{E}_i^0} \underline{E}_{ji} \right\}$
- DD partition: $W_i(\Omega_i') = W_i(I_i) \times W_i(\Gamma_i')$
- Product spaces:

$$W(\Omega') := \prod_{i=0}^{N} W_i(\Omega_i'), \qquad W(\Gamma') := \prod_{i=0}^{N} W_i(\Gamma_i'),$$

- "Different" continuity concept

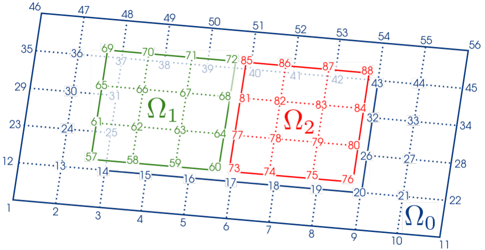


M Dryja, J Galvis and M Sarkis, *J. Complexity* (2007).



Suppose $\tau = 1$

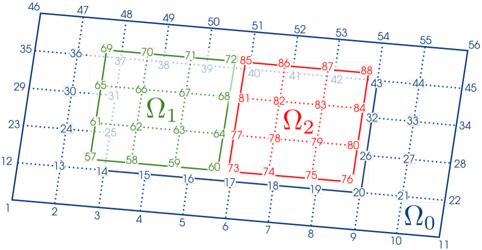
$$K = \left[\begin{array}{cc:cc:cc}
A_{I_0 I_0} & A_{I_0 \Gamma_0} & & & & \\
A_{\Gamma_0 I_0} & A_{\Gamma_0 \Gamma_0} + M_{\Gamma_0 \Gamma_0} & & -M_{\Gamma_0 \Gamma_1} & & -M_{\Gamma_0 \Gamma_2} \\
\hdashline
 & & A_{I_1 I_1} & A_{I_1 \Gamma_1} & & \\
 & -M_{\Gamma_1 \Gamma_0} & A_{\Gamma_1 I_1} & A_{\Gamma_1 \Gamma_1} + M_{\Gamma_1 \Gamma_1} & & -M_{\Gamma_1 \Gamma_2} \\
\hdashline
 & & & & A_{I_2 I_2} & A_{I_2 \Gamma_2} \\
 & -M_{\Gamma_2 \Gamma_0} & & -M_{\Gamma_2 \Gamma_1} & A_{\Gamma_2 I_2} & A_{\Gamma_2 \Gamma_2} + M_{\Gamma_2 \Gamma_2}
\end{array}\right]$$



Local contributions are given by

$$
K_0' = \left[\begin{array}{cc:c:c}
A_{I_0 I_0} & A_{I_0 \Gamma_0} & & \\
A_{\Gamma_0 I_0} & A_{\Gamma_0\Gamma_0} + \frac{1}{2} M_{\Gamma_0\Gamma_0} & -\frac{1}{2} M_{\Gamma_0\Gamma_1} & -\frac{1}{2} M_{\Gamma_0\Gamma_2} \\
\hdashline
 & -\frac{1}{2} M_{\Gamma_1\Gamma_0} & \frac{1}{2} M^{10}_{\Gamma_1\Gamma_1} & \\
\hdashline
 & -\frac{1}{2} M_{\Gamma_2\Gamma_0} & & \frac{1}{2} M^{20}_{\Gamma_2\Gamma_2}
\end{array}\right],
$$

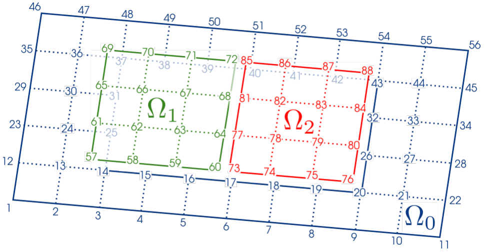
$$
M_{\Gamma_0\Gamma_0} = M^{01}_{\Gamma_0\Gamma_0} + M^{02}_{\Gamma_0\Gamma_0}, \qquad M_{\Gamma_1\Gamma_1} = M^{10}_{\Gamma_1\Gamma_1} + M^{12}_{\Gamma_1\Gamma_1}, \qquad M_{\Gamma_2\Gamma_2} = M^{20}_{\Gamma_2\Gamma_2} + M^{21}_{\Gamma_2\Gamma_2}.
$$



Local contributions are given by

$$K_1' = \left[\begin{array}{c:cc:c} \frac{1}{2} M^{01}_{\Gamma_0\Gamma_0} & & -\frac{1}{2} M_{\Gamma_0\Gamma_1} & \\ \hdashline & A_{I_1I_1} & A_{I_1\Gamma_1} & \\ -\frac{1}{2} M_{\Gamma_1\Gamma_0} & A_{\Gamma_1 I_1} & A_{\Gamma_1\Gamma_1} + \frac{1}{2} M_{\Gamma_1\Gamma_1} & -\frac{1}{2} M_{\Gamma_1\Gamma_2} \\ \hdashline & & -\frac{1}{2} M_{\Gamma_2\Gamma_1} & \frac{1}{2} M^{21}_{\Gamma_2\Gamma_2} \end{array}\right],$$

$$M_{\Gamma_0\Gamma_0} = M^{01}_{\Gamma_0\Gamma_0} + M^{02}_{\Gamma_0\Gamma_0}, \qquad M_{\Gamma_1\Gamma_1} = M^{10}_{\Gamma_1\Gamma_1} + M^{12}_{\Gamma_1\Gamma_1}, \qquad M_{\Gamma_2\Gamma_2} = M^{20}_{\Gamma_2\Gamma_2} + M^{21}_{\Gamma_2\Gamma_2}.$$



Local contributions are given by

$$K_2' = \left[\begin{array}{c:c:cc} & & & \\ \frac{1}{2}\textcolor{teal}{M^{02}_{\Gamma_0\Gamma_0}} & & & -\frac{1}{2}M_{\Gamma_0\Gamma_2} \\ \hdashline & & & \\ & \frac{1}{2}\textcolor{teal}{M^{12}_{\Gamma_1\Gamma_1}} & & -\frac{1}{2}M_{\Gamma_1\Gamma_2} \\ \hdashline & & A_{I_2I_2} & A_{I_2\Gamma_2} \\ -\frac{1}{2}M_{\Gamma_2\Gamma_0} & -\frac{1}{2}M_{\Gamma_2\Gamma_1} & A_{\Gamma_2I_2} & A_{\Gamma_2\Gamma_2}+\frac{1}{2}M_{\Gamma_2\Gamma_2} \end{array}\right].$$

$$M_{\Gamma_0\Gamma_0} = M^{01}_{\Gamma_0\Gamma_0} + \textcolor{teal}{M^{02}_{\Gamma_0\Gamma_0}}, \qquad M_{\Gamma_1\Gamma_1} = M^{10}_{\Gamma_1\Gamma_1} + \textcolor{teal}{M^{12}_{\Gamma_1\Gamma_1}}, \qquad M_{\Gamma_2\Gamma_2} = M^{20}_{\Gamma_2\Gamma_2} + M^{21}_{\Gamma_2\Gamma_2}.$$

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- Reordered "fat" local matrix $\mathcal{K}'_i$

$$\mathcal{K}'_i = \begin{bmatrix} K'_{i,II} & K'_{i,I\Gamma'} \\ K'_{i,\Gamma' I} & K'_{i,\Gamma'\Gamma'} \end{bmatrix} = \begin{bmatrix} K'_{i,II} & K'_{i,I\Delta} & K'_{i,I\Pi} \\ K'_{i,\Delta I} & K'_{i,\Delta\Delta} & K'_{i,\Delta\Pi} \\ K'_{i,\Pi I} & K'_{i,\Pi\Delta} & K'_{i,\Pi\Pi} \end{bmatrix}.$$

- Two level preconditioner for the Schur complement system $\widehat{S}_{\Gamma'} u_{\Gamma'} = \widehat{f}_{\Gamma'}$:

$$M^{-1}_{\mathrm{BDDC}} = \widetilde{R}^T_{D,\Gamma'} (\widetilde{S}_{\Gamma'})^{-1} \widetilde{R}_{D,\Gamma'}, \qquad \widetilde{S}_{\Gamma'} = \widetilde{R}_{\Gamma'} S' \widetilde{R}^T_{\Gamma'}. \tag{1}$$

- The action of $\widetilde{S}^{-1}_{\Gamma'}$ can be evaluated with

$$\widetilde{S}^{-1}_{\Gamma'} = \widetilde{R}^T_{\Gamma\Delta} \left(\sum_{i=0}^{N} \begin{bmatrix} 0 & R^T_{i,\Delta} \end{bmatrix} \begin{bmatrix} K'_{i,II} & K'_{i,I\Delta} \\ K'_{i,\Delta I} & K'_{i,\Delta\Delta} \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ R_{i,\Delta} \end{bmatrix} \right) \widetilde{R}_{\Gamma'\Delta} + \Phi S^{-1}_{\Pi\Pi} \Phi.$$

  - Sum of local solvers on each subdomain Ω'_i with Neumann data on Δ and zero value on primal dofs;
  - Coarse solver for the primal variables
    - Φ maps the primal dofs Π to the interface variables Γ
    - $S_{\Pi\Pi}$ represent the primal problem

Lemma

Let the primal set be spanned by the vertex nodal finite element functions and let $h = \mathcal{O}(\tau)$. If the projection operator is scaled by the ρ-scaling, then $\forall u \in \widetilde{W}(\Gamma')$

$$|P_D u|^2_{S'} \leq C\,\Psi(\tau, h)\left(1 + \log\frac{H}{h}\right)^2 |u|^2_{S'}$$

with C constant independent of all the parameters of the problem and with

$$\Psi(\tau, h) = 1 + \frac{2\,\sigma_M}{C_m}\frac{\tau}{h},$$

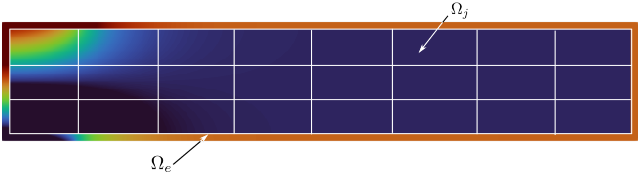
where σ_M is the maximum value of σ_i over all the subdomains, τ the time step size and h the mesh size.

Theoretical limitation

The hypothesis of $h = \mathcal{O}(\tau)$ is needed since $\Psi(\tau, h)$ can grow uncontrolled when the mesh size decreases, i.e. $h \to 0$.

NMMH, F Chegini, LF Pavarino, M Weiser, S Scacchi, *arXiv preprint:2212.12295* (2022).

Matlab setting



- 2D rectangular geometry
- Aliev-Panfilov ionic model
- time interval $[0, 5]$ ms
- fixed $\tau = 0.05$ ms
- applied current of 50 mA/cm^2

- Linear gap junctions $G(v) = \frac{v}{R}$
- Ω_e frames the myocites
- Iterative solver: Conjugate Gradient (CG)
- Preconditioners for Schur system: *BDDCSchur*, no preconditioning (*NoPCSchur*)
- Additional solver: CG for the full problem (NoPCFull)
- Performed on office workstation: 18 Intel cores i9-10980XE CPU 3.00 GHz

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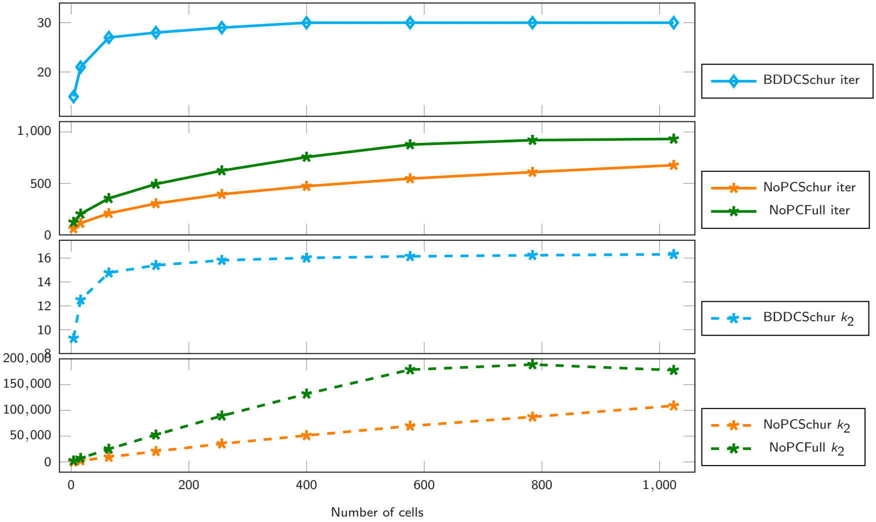
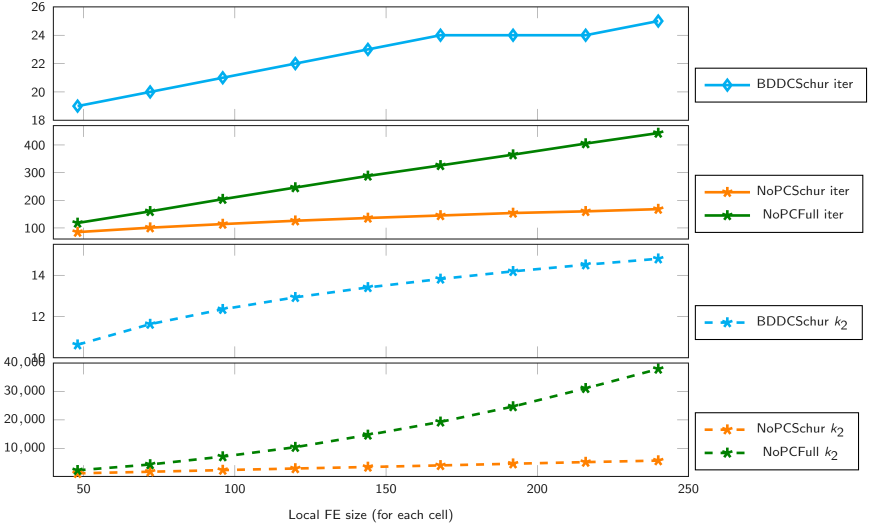
Matlab scalability and optimality



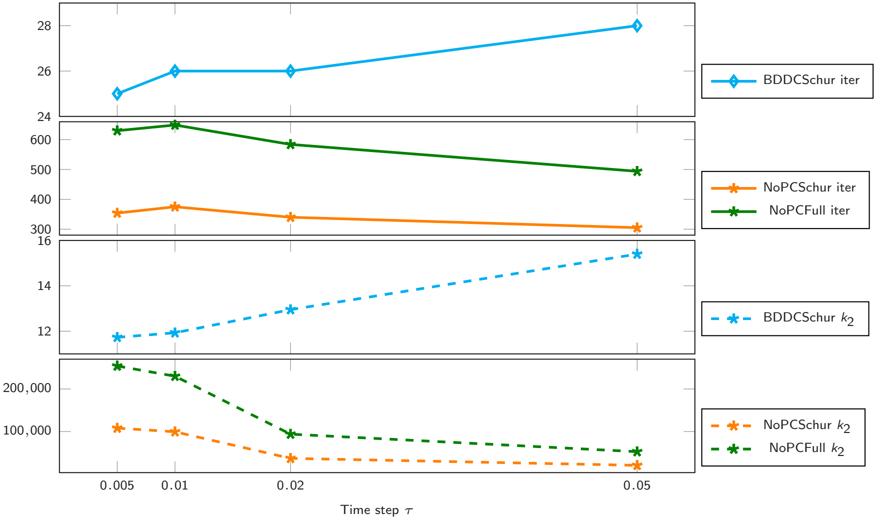
Scalability: fixed local size (24 × 4 FE), increasing number of myocytes (from 4 to 1024).
Biggest case with more than 100k DoFs.

Matlab scalability and optimality



Optimality: fixed number of myocytes (16), increasing local FE size (from 48 to 240).

Matlab - dependence on time step



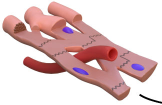
Fixed number of myocytes (16), each discretized with 24×4 FEs.

Let's summarize!

- ◇ Standard finite element discretizations keep these natural discontinuities
- ◇ A model-based non-overlapping DD preconditioner (BDDC) has been designed
  - "fat" local interface spaces
  - different concept of continuity
  - proof of theoretical convergence

NMMH, F Chegini, LF Pavarino, M Weiser, S Scacchi, *arXiv preprint:2212.12295* (2022)

- ◇ Extensive 2-dimensional tests prove scalability and optimality



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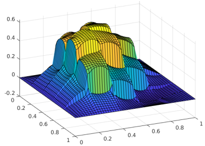

Microscopic model — Algebraic system — Model-based Domain Decomposition solver

Let's summarize!

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- ◇ Extensive 2-dimensional tests prove scalability and optimality

What's next?

- ◇ Validation of the proposed solver to 3-dimensional settings
- ◇ Investigation of other DD preconditioners to such settings