High performance computing in computational electrocardiology II: scalable solvers

Simone Scacchi University of Milan, Italy

Joint work with

Piero Colli Franzone University of Pavia, Italy
Luca F. Pavarino University of Milan, Italy
Stefano Zampini KAUST, Saudi Arabia

MHPC Workshop on High Performance Computing
February 24-26 2016, SISSA, Trieste

The cardiac electromechanical coupling model: summary of equations

$$
\begin{cases}
\dfrac{\partial w}{\partial t} = R(v, w) \\
\dfrac{\partial c}{\partial t} = S(v, w, c) \\
\dfrac{d\mathbf{z}}{dt} = \mathbf{R}_z\left(\mathbf{z}, [Ca^{2+}]_i, T_a, \lambda, \dfrac{d\lambda}{dt}\right) \\
T_a = T_a(\mathbf{z}, \lambda) \\
\mathrm{div}(\mathbf{FS}) = 0 \\
c_m \dfrac{\partial v}{\partial t} - \dfrac{1}{\det(\mathbf{F})} \mathrm{div}(\det(\mathbf{F})\mathbf{F}^{-1} D_i \mathbf{F}^{-T} \nabla u_i) + I_{ion}(v, w, c) = 0 \\
-c_m \dfrac{\partial v}{\partial t} - \dfrac{1}{\det(\mathbf{F})} \mathrm{div}(\det(\mathbf{F})\mathbf{F}^{-1} D_e \mathbf{F}^{-T} \nabla u_e) - I_{ion}(v, w, c) = I^e_{app}
\end{cases}
$$

Space and time discretization

Space discretization: isoparametric Q^1 finite elements

Time discretization: splitting method

1- given v^n, w^n, c^n, solve the ODEs of the membrane model with a first order IMEX method to compute the new w^{n+1}, c^{n+1}

2- given Ca_i^{n+1} solve the active tension model and the finite elasticity system to compute the new deformed coordinates $\mathbf{x}^{n+1}$, providing the new deformation gradient tensor $\mathbf{F}^{n+1}$

3- given w^{n+1}, c^{n+1}, $\mathbf{F}^{n+1}$ solve the Bidomain system with a first order IMEX method computing the new electric potentials u_i^{n+1}, u_e^{n+1}, $v^{n+1} = u_i^{n+1} - u_e^{n+1}$

Time discretization of mechanical components

At each time step:
given the calcium concentration Ca_i^{n+1}, solve the non-linear elasticity equations coupled with the active tension model

$$\begin{cases} \mathbf{z}^{n+1} = \mathbf{z}^n + \Delta t R_z \left(\mathbf{z}^{n+1}, Ca_i^{n+1}, \lambda^{n+1}, \dfrac{\lambda^{n+1} - \lambda^n}{\Delta t_n} \right) \\ T_a^{n+1} = f_{Ta}(\mathbf{z}^{n+1}, \lambda^{n+1}) \\ \mathrm{div}(\mathbf{F}_{n+1}\mathbf{S}_{n+1}) = 0, \end{cases}$$

with

$$\mathbf{S}_{n+1} = \mathbf{S}^{pas}(\mathbf{F}_{n+1}) + \mathbf{S}^{vol}(\mathbf{F}_{n+1}) + \mathbf{S}^{act}(\mathbf{F}_{n+1}, T_a^{n+1}).$$

Mechanical and Bidomain solvers

At each time step, the main computational effort consists of

1- solving the non-linear system deriving from the discretization of the mechanical problem. We use the Newton method, with GMRES for the Jacobian system, preconditioned by an Algebraic Multigrid preconditioner (BoomerAMG, Henson and Yang, 2002)

2- solving the linear system deriving from the discretization of the Bidomain model. We use the Conjugate Gradient method preconditioned by the Multilevel Additive Schwarz preconditioner

Literature on Mechanical and Bidomain solvers

Mechanical solvers:

- Newton+parallel direct solvers for the Jacobian (Vetter and McCulloch 2000, Gurev et al. 2011),
- Newton+parallel AMG for the Jacobian (Colli Franzone, Pavarino, S. 2015, Augustin et al. 2016).
- Newton+BDDC for the Jacobian (Pavarino, S., Zampini 2015)

Bidomain solvers:

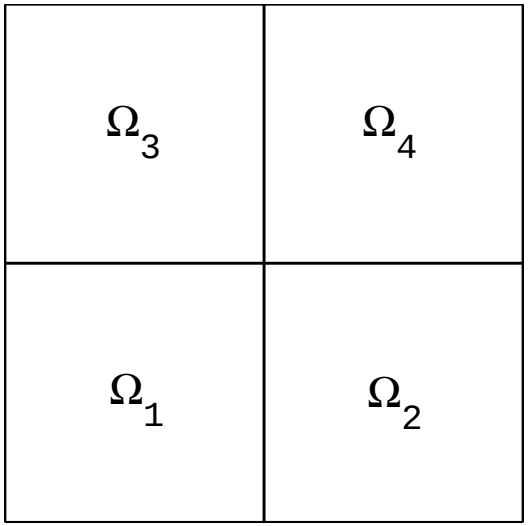
- AMG (Plank et al. 2007, Pennacchio, Simoncini, 2009),
- Block Triangular (Gerardo Giorda et al. 2009),
- Block Jacobi (Colli Franzone, Pavarino, 2004),
- Additive Schwarz (Pavarino, S., 2008),
- Neumann-Neumann, BDDC (Zampini, 2013, 2014)

Overlapping Additive Schwarz preconditioner: the subdomains partition

Consider the variational problem

$$\text{find } u_h \in V_h : \quad a(u_h, v) = (f, v) \quad \forall v \in V_h.$$

The first step is to divide the parametric space into N non-overlapping subdomains Ω_i of diameter H.

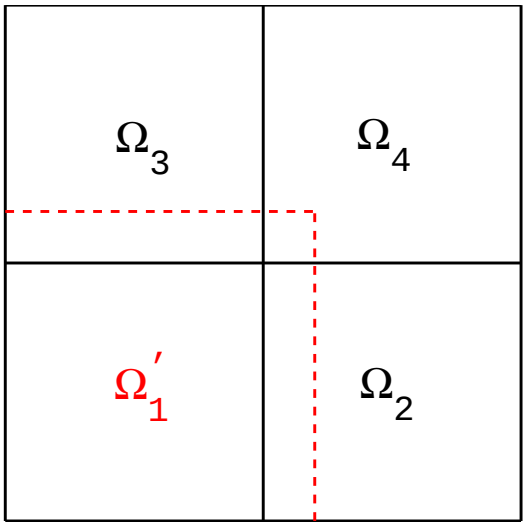


Overlapping Additive Schwarz preconditioner: the subdomains partition

Consider the variational problem

$$\text{find } u_h \in V_h : \quad a(u_h, v) = (f, v) \quad \forall v \in V_h.$$

Then extend each subdomain to obtain a partition of the parametric space into N overlapping subdomains Ω_i'.
Let δ be the overlap parameter.



One-level Additive Schwarz preconditioner: the operator construction

- Introduce the local FEM spaces related to subdomains

$$V_i := \{\mathbf{v} \in V_h \,:\, \mathbf{v}(x) = 0 \; x \in \Omega \backslash \Omega_i'\}, \quad i = 1, ..., N$$

- Define the projections $\mathbf{T}_i : V_h \rightarrow V_i,\ i = 1, ..., N$

$$a(\mathbf{T}_i \mathbf{u}, \mathbf{v}) = a(\mathbf{u}, \mathbf{v}) \quad \forall \mathbf{v} \in V_i.$$

- The one-level Additive Schwarz operator is given by

$$\mathbf{T}_{AS1} = \mathbf{T}_1 + ... + \mathbf{T}_N = P_{AS1}^{-1} A.$$

where P_{AS1}^{-1} is the one Additive Schwarz preconditioner and A the original stiffness matrix.

One-level Additive Schwarz preconditioner: convergence rate

Theorem

The condition number of the one-level additive Schwarz preconditioned operator $\mathbf{T}_{AS1}$ *is bounded by*

$$\kappa_2(\mathbf{T}_{AS1}) \leq C \frac{1}{H^2} \left(1 + \frac{H}{\delta}\right),$$

where δ *is the overlap parameter and* C *is a constant independent of* h, H, N, δ.

Toselli-Widlund 2004

Two-level Additive Schwarz preconditioner: the operator construction

- Introduce the local FEM spaces related to subdomains

$$V_i := \{\mathbf{v} \in V_h \,:\, \mathbf{v}(x) = 0 \; x \in \Omega \backslash \Omega_i'\}, \quad i = 1, ..., N$$

- Introduce the coarse FEM space

$$V_0 \subset V_h$$

- Define the projections $\mathbf{T}_i : V_h \to V_i$, $i = 0, ..., N$

$$a(\mathbf{T}_i \mathbf{u}, \mathbf{v}) = a(\mathbf{u}, \mathbf{v}) \quad \forall \mathbf{v} \in V_i.$$

- The two-level Additive Schwarz operator is given by

$$\mathbf{T}_{AS2} = \mathbf{T}_0 + \mathbf{T}_1 + ... + \mathbf{T}_N = P_{AS2}^{-1} A.$$

where P_{AS2}^{-1} is the two-level Additive Schwarz preconditioner and A the original stiffness matrix.

Two-level Additive Schwarz preconditioner: convergence rate

Theorem

The condition number of the two-level additive Schwarz preconditioned operator $\mathbf{T}_{OAS}$ *is bounded by*

$$\kappa_2(\mathbf{T}_{AS2}) \leq C\left(1+\frac{H}{\delta}\right),$$

where δ *is the overlap parameter and* C *is a constant independent of* h, H, N, δ.

Toselli-Widlund 2004

Multilevel Additive Schwarz preconditioner for the Bidomain system: convergence rate

Theorem

The condition number of the L-level Additive Schwarz (MAS(L)) preconditioned operator $\mathbf{T}_{MAS}$ *is bounded by*

$$\kappa_2(\mathbf{T}_{MAS}) \leq C \max_{k=1,\ldots,L-1} \left(1 + \frac{H_{k-1}}{\delta_k}\right)$$

where C *is independent of*

- $L =$ *number of levels,*
- $H_k =$ *size of subdomains at level* k*,*
- $\delta_k =$ *overlap at level* k *.*

Pavarino, S. SIAM J Sci Comput, 2008

Parallel implementation

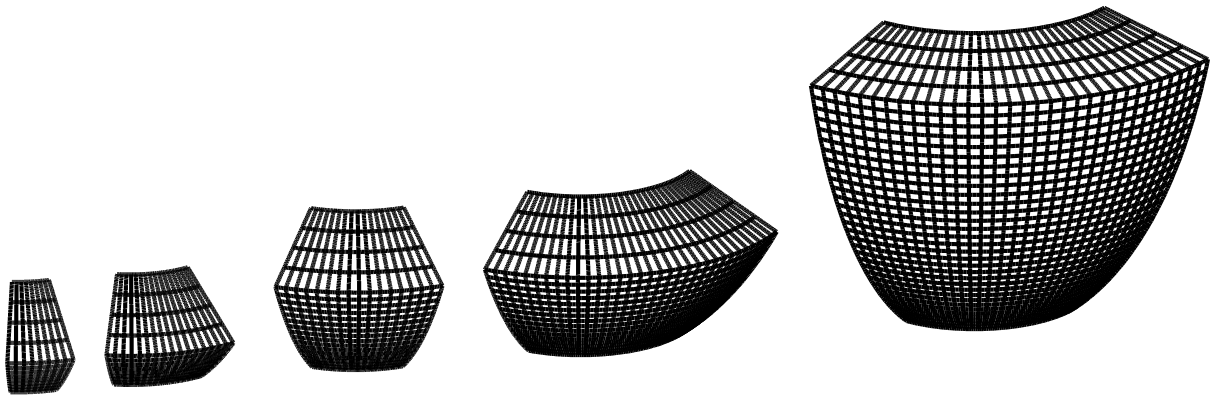
- FORTRAN 90 code
- Based on:
  1- MPI library
  2- PETSc library (Argonne National Laboratory)
  3- BoomerAMG provided within the HYPRE library (Lawrence Livermore National Laboratory)
- Computational platforms:
  - IBM BlueGene/Q of CINECA (163 840 cores)
  - IBM BlueGene/Q of Argonne National Laboratory (786 432 cores)

Bidomain parallel results: weak scalability, comparison MAS(4) vs. AS1

40 time steps, $\Delta t = 0.05$ ms.

κ_2 = condition number of the preconditioned system

it = PCG iterations



256 512 1024 2048 4096

		AS1 prec.			MAS(4) prec.		
procs	dofs	κ_2	it	time (s)	κ_2	it	time (s)
64	4.3e+6	8.10e+3	233	4.84	12.34	23	1.24
128	8.5e+6	8.02e+3	268	5.65	12.33	23	1.35
256	1.7e+7	2.69e+4	342	7.32	11.43	22	1.43
512	3.3e+7	2.65e+4	414	9.01	11.42	22	1.54
1024	6.7e+7	4.53e+4	523	11.26	11.43	22	1.69

Bidomain parallel results: weak scalability

4-level Additive Schwarz preconditioner

overlap $\delta = h$, ILU(0) local solvers

local mesh size 32^3 (+ overlap), 10 time steps, $\Delta t = 0.05$ ms.

κ_2 = condition number of the preconditioned system

it = PCG iterations

run on Bluegene/Q of CINECA

procs	dofs	$\kappa_2 = \lambda_M/\lambda_m$	it	time (s)
64	4.3e+6	15.5=4.5/2.9e-1	29	1.8
128	8.5e+6	14.9=4.5/3.0e-1	28	2.0
256	1.7e+7	15.4=4.5/2.9e-1	28	1.9
512	3.3e+7	14.3=4.4/3.0e-1	28	2.0
1024	6.7e+7	14.4=4.4/3.1e-1	28	2.2
2048	1.3e+8	13.2=4.3/3.3e-1	27	2.9
4096	2.7e+8	13.2=4.3/3.3e-1	27	5.6
8192	5.4e+8	12.4=4.3/3.5e-1	26	5.9
16384	1.1e+9	12.4=4.3/3.5e-1	26	6.2
32768	2.1e+9	12.0=4.3/3.6e-1	26	6.9

Bidomain parallel results: weak scalability

4-level Additive Schwarz preconditioner

overlap $\delta = h$, ILU(0) local solvers

local mesh size 16^3 (+ overlap), 10 time steps, $\Delta t = 0.05$ ms.

κ_2 = condition number of the preconditioned system

it = PCG iterations

run on Bluegene/Q of Argonne National Laboratory

procs	dofs	$\kappa_2 = \lambda_M/\lambda_m$	it	time (s)
1024	4 293 185	6.40=4.06/0.63	12	0.62
2048	8 569 665	8.33=4.27/0.51	14	1.11
4096	17 105 985	10.51=4.24/0.40	15	1.27
8192	33 948 801	6.33=4.00/0.63	12	1.02
16384	67 831 425	8.60=4.43/0.51	14	1.73
32768	135 530 625	10.41=4.25/0.41	15	1.80
65536	270 010 625	5.94=4.00/0.67	10	1.36
131072	539 757 825	7.23=4.38/0.61	10	1.95
163840	674 631 425	8.35=4.72/0.57	10	3.28

Weak scaling test: robustness of Bidomain solver with respect to deformation

Fixed local Bidomain dofs per subdomain 68 656

Bidomain solver - MHS(4) preconditioner							
		non-deforming ($\mathbf{C} = \mathbf{I}$)			deforming		
procs	dofs	κ_2	it	time	κ_2	it	time
8	549 250	1.11	3	1.05	1.11	3	1.31
27	1 825 346	1.11	3	1.19	1.12	3	1.17
64	4 293 378	1.12	3	1.23	1.13	3	1.21
125	8 346 562	1.13	3	1.31	1.18	4	1.49
216	14 378 114	1.18	4	1.55	1.20	4	1.55
343	22 781 250	1.15	4	1.62	1.17	4	1.66
512	33 949 186	1.14	4	1.96	1.17	4	1.67

κ_2 = average condition number per time step

it = average CG iteration counts per time step

time = average CPU time in seconds to solve one Bidomain linear system

Mechanical solver: AMG strong scalability

Fixed global mechanical dofs: 823 872

Mechanical solver - AMG preconditioner					
procs	local dofs	nit	lit	time	speedup
8	102 984	2	41	110.84	-
16	51 492	2	40	63.61	1.74 (2)
32	25 746	2	41	34.64	3.20 (4)
64	12 873	2	39	23.26	4.76 (8)
128	6 436	2	40	16.08	6.89 (16)
256	3 218	2	40	15.50	7.15 (32)
512	1 609	2	41	16.97	6.53 (64)

nit = Newton iterations

it = CG iteration counts

time = CPU time in sec. to solve mechanical pb.

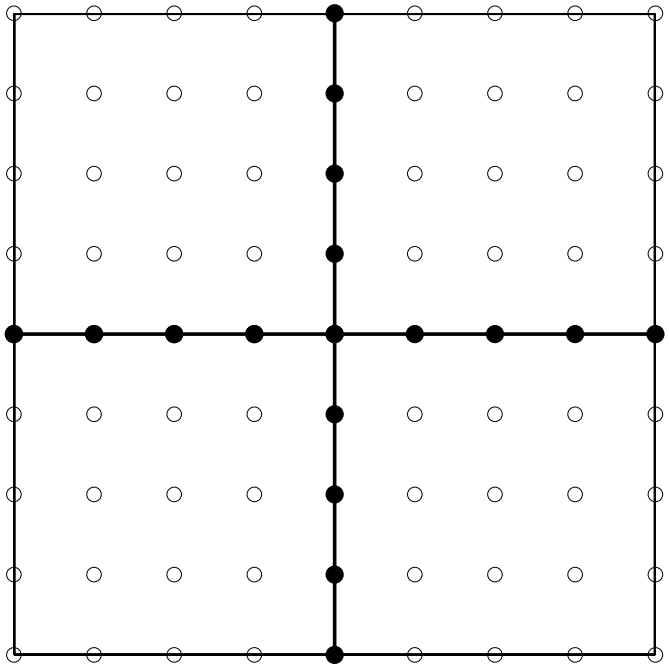
Weak scaling test: mechanical solver

- Simulation of 1.5 *ms* (30 time steps of $\tau = 0.05$ *ms*) during the plateau phase on truncated ellipsoidal domains.
- Fixed local mechanical dofs per subdomain 13 476

Mechanical solver - AMG preconditioner				
procs	dofs	Newton iter.	GMRES iter.	CPU time
8	107 811	2	42	12.06
27	352 947	2	42	16.70
64	823 875	2	39	23.45
125	1 594 323	2	39	30.66
216	2 738 019	2	40	49.12
343	4 328 691	2	39	92.93
512	6 440 067	2	40	75.09

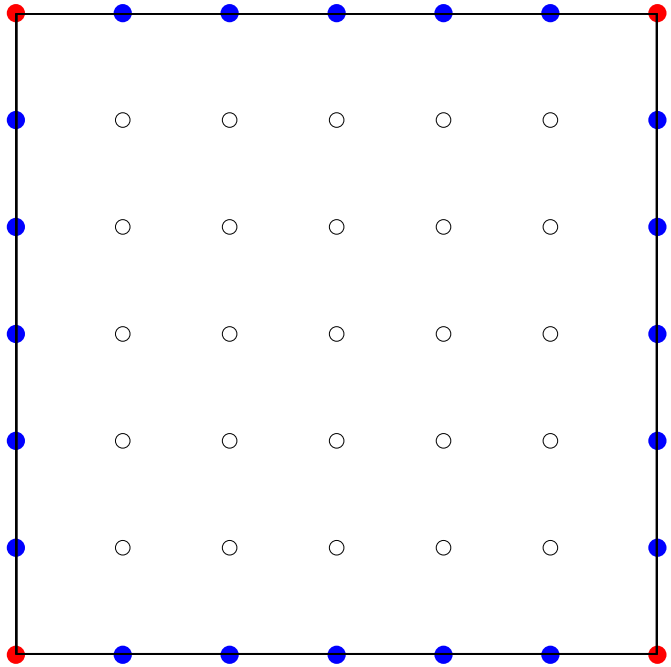
Mechanical solvers: the BDDC preconditioner I

The Balancing Domain Decomposition by Constraints (BDDC) preconditioner, introduced by Dohrmann 2003, is a preconditioner for the Schur Complement system, obtained eliminating by static condensation the unknowns interior to the subdomains.



Mechanical solvers: the BDDC preconditioner II

Subdivide then the interface unknowns into primal and dual



- The primal unknowns are the solution of a global coarse problem.
- The dual unknowns are the solution of independent local problems with mixed boundary conditions, Dirichlet on the primal and Neumann on the dual

BDDC preconditioner: convergence rate

Theorem

In case symmetric positive definite problems (elliptic equations, compressible linear elasticity), the condition number of the BDDC preconditioned operator $\mathbf{T}_{BDDC}$ *is bounded by*

$$\kappa_2(\mathbf{T}_{BDDC}) \leq C \left(1 + \log\left(\frac{H}{h}\right)\right)^2,$$

where C *is a constant independent of*

- h *fine mesh size,*
- H *coarse mesh size,*
- N *number of subdomains.*

Mandel and Dohrmann 2003

Mechanical solvers: BDDC strong scalability

Fixed global mesh on ellipsoidal domain: $385 \times 385 \times 97$

BDDC primal constraints: VE = Vertex + Edges aver.

VEF = Vertex + Edges aver.+ Faces aver.

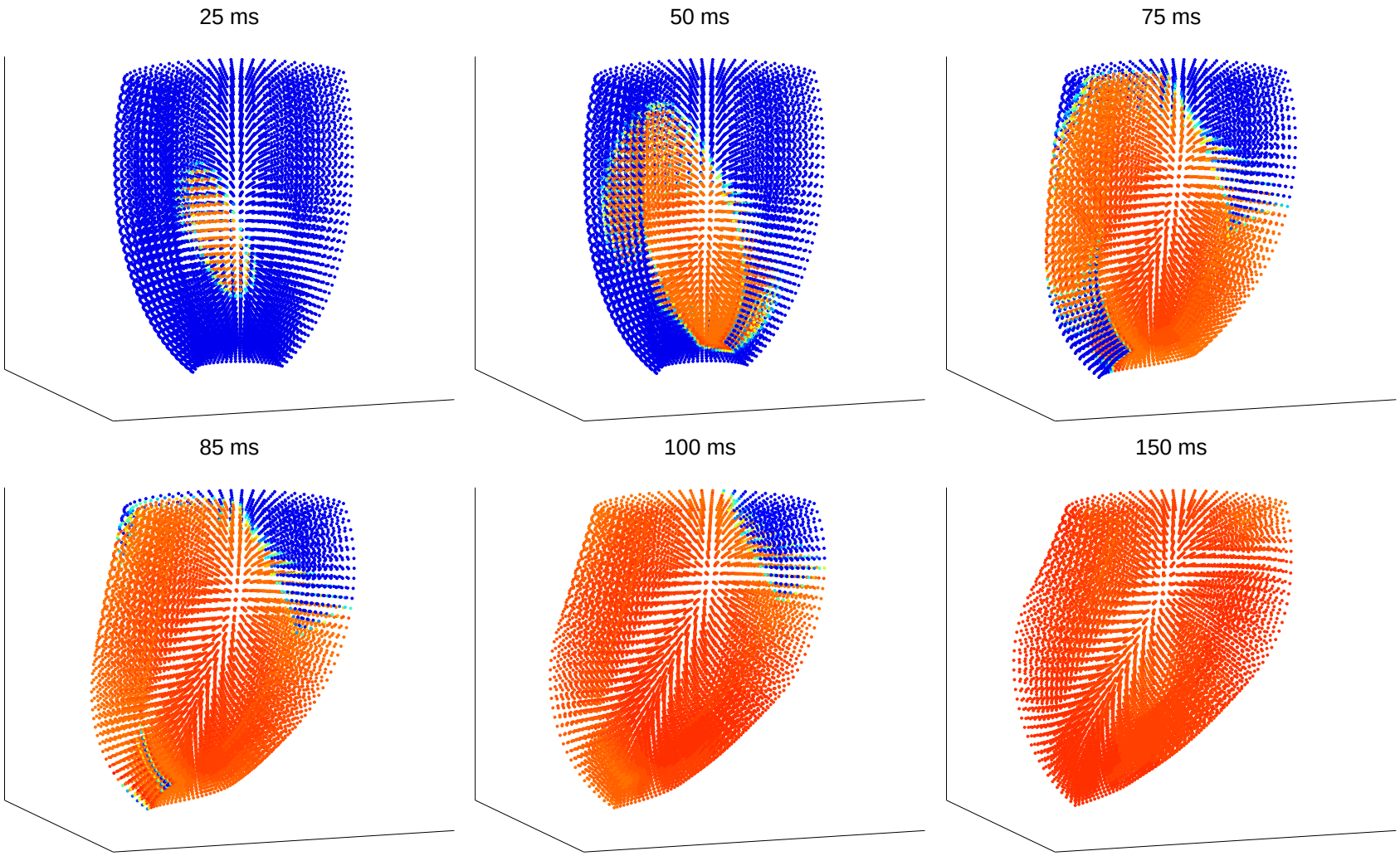
Mechanical solver - BDDC preconditioner									
	VE			VEF			boomerAMG		
procs	nit	lit	time	nit	lit	time	nit	lit	time
64	2	58	80.1	2	57	82.9	2	80	30.6
128	2	53	28.9	2	47	29.8	2	80	20.7
256	2	88	11.4	2	75	11.6	2	81	14.6
512	2	87	5.5	2	75	5.7	2	79	15.4
1024	2	59	3.7	2	43	3.7	2	80	28.8

Mechanical solvers: BDDC weak scalability

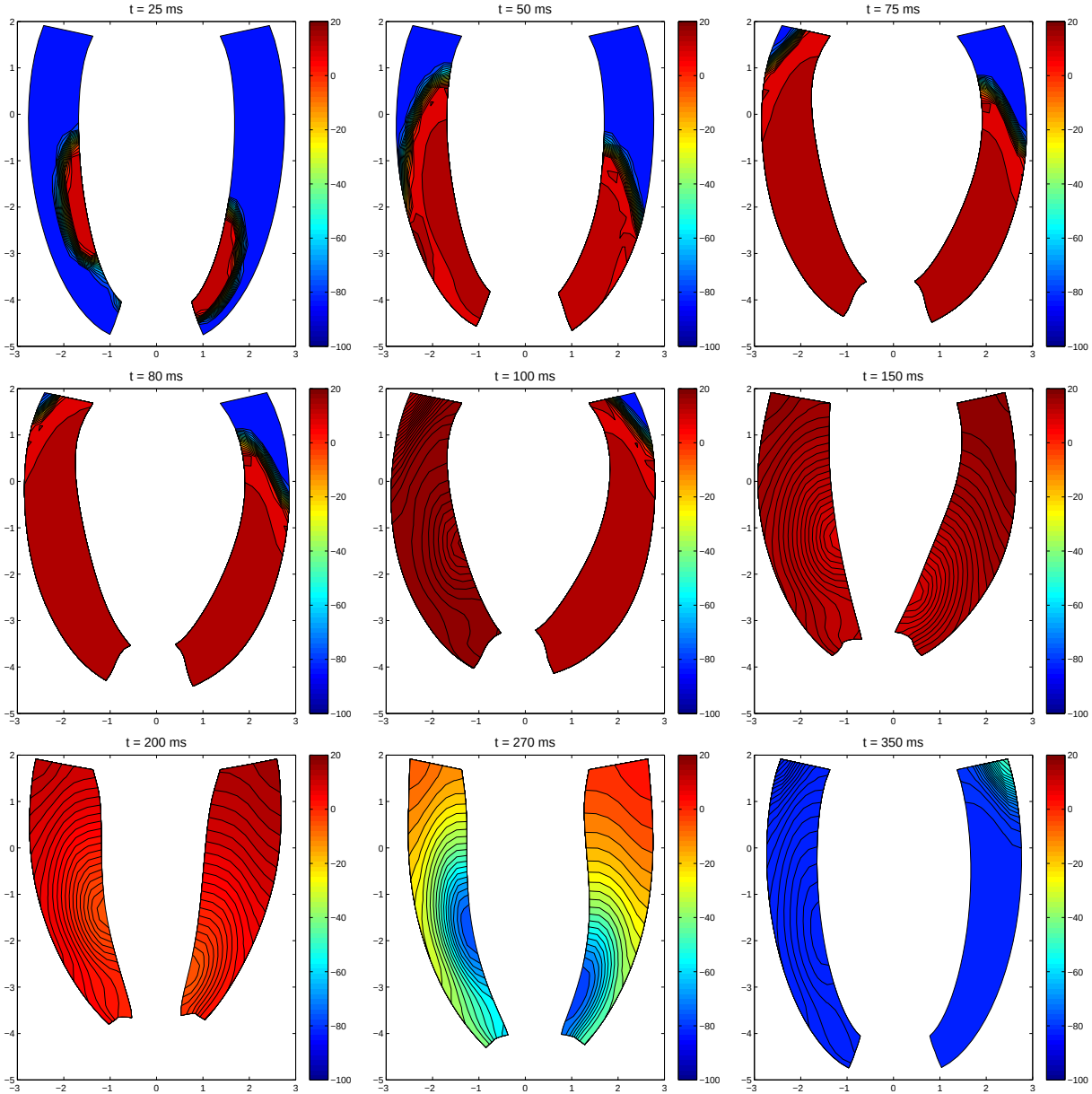
Fixed local mesh on slab domain: $20 \times 20 \times 20$
BDDC primal dofs: V = Vertexes
VE = Vertexes + Edge averages
run on Bluegene/Q of Cineca

		V			VE		
procs	dofs	nit	lit	time (s)	nit	lit	time (s)
256	105 903	2	473	0.74	2	165	0.81
512	209 223	2	566	1.50	2	185	1.14
1024	413 343	2	598	2.15	2	177	1.67
2048	807 003	2	644	3.11	2	180	2.63
4096	1 633 023	2	589	5.00	2	181	4.17
8192	3 188 283	2	626	28.33	2	192	7.89
16384	6 491 583	2	796	33.24	2	189	14.06

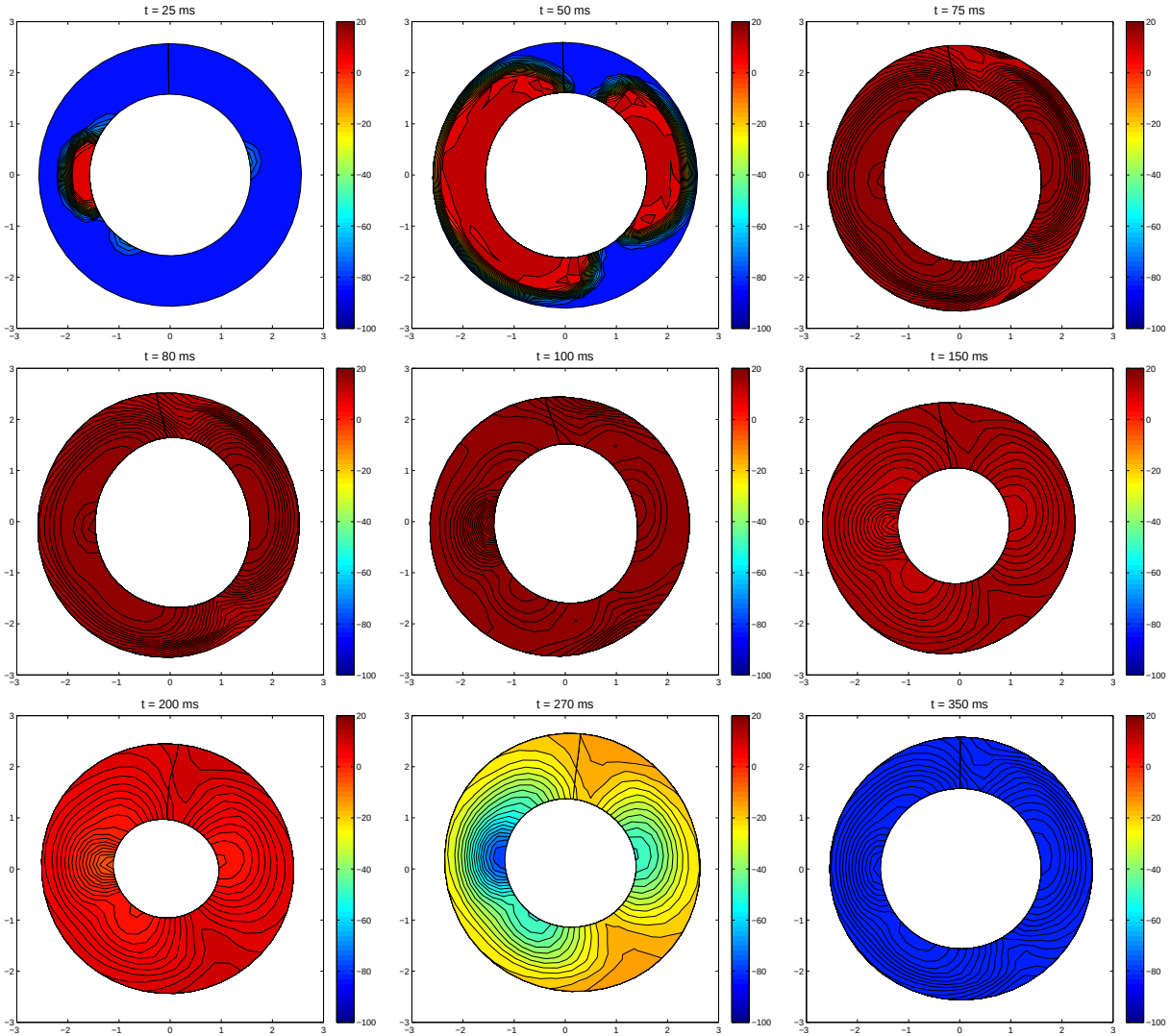
Full cardiac cycle simulation



Full cardiac cycle simulation: longitudinal sections



Full cardiac cycle simulation: circumferential sections



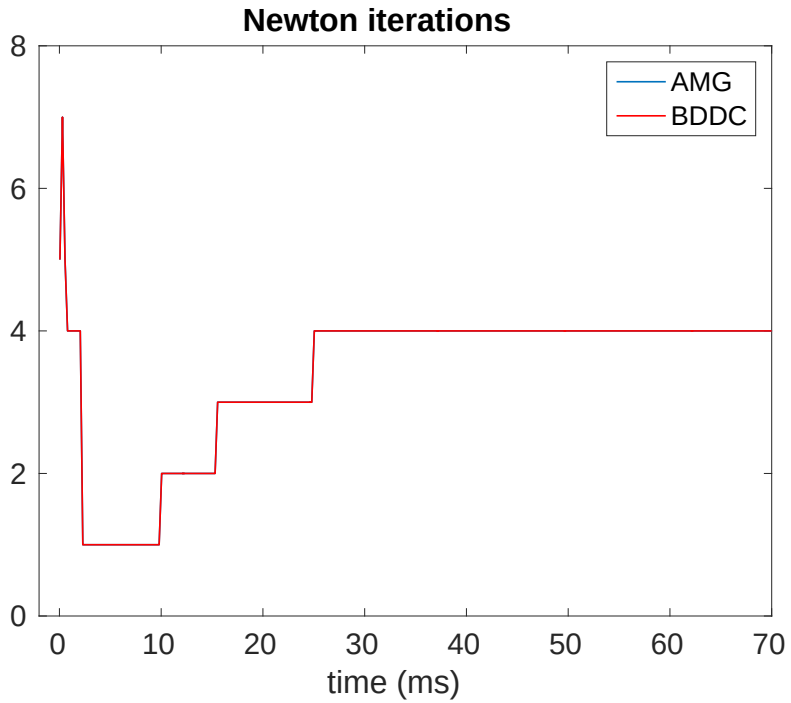
Comparison BDDC vs. AMG on the simulation of the excitation-contraction process

Simulation of 70 ms of ventricular excitation-contraction process
Closed truncated ellipsoidal domain
Electrical mesh: 25 692 290 dofs, Mechanical mesh: 86 427 dofs
run on 256 processors of Bluegene/Q of CINECA

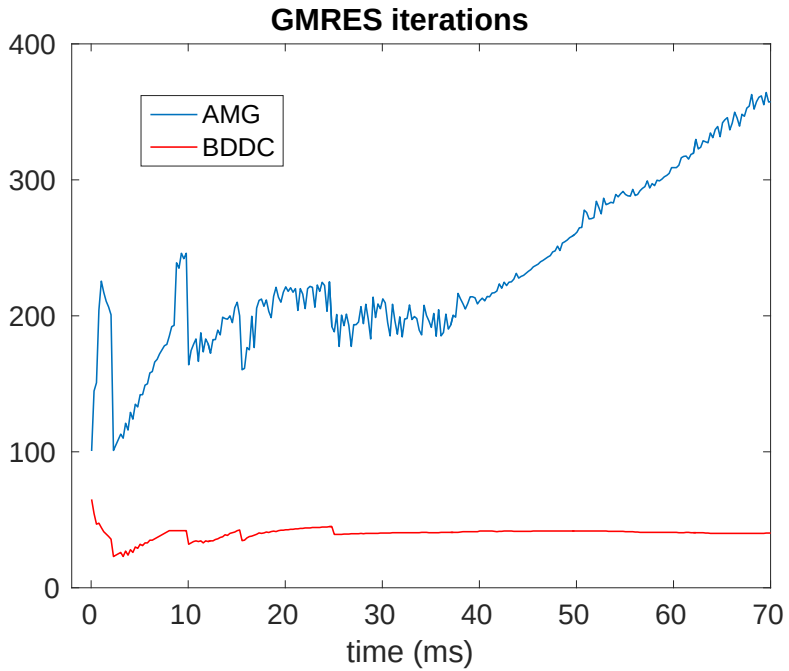
prec	Tnit	nit	Tlit	lit	Ttime (s)	time (s)
AMG	6790	3	1642220	232	64578	32.29
BDDC	6790	3	276932	40	6083	3.04

Total (Tnit) and average per time step (nit) Newton iterations
Total (Tlit) and average per Newton iteration (lit) GMRES iterations
Total (Ttime) and average per time step (time) CPU times

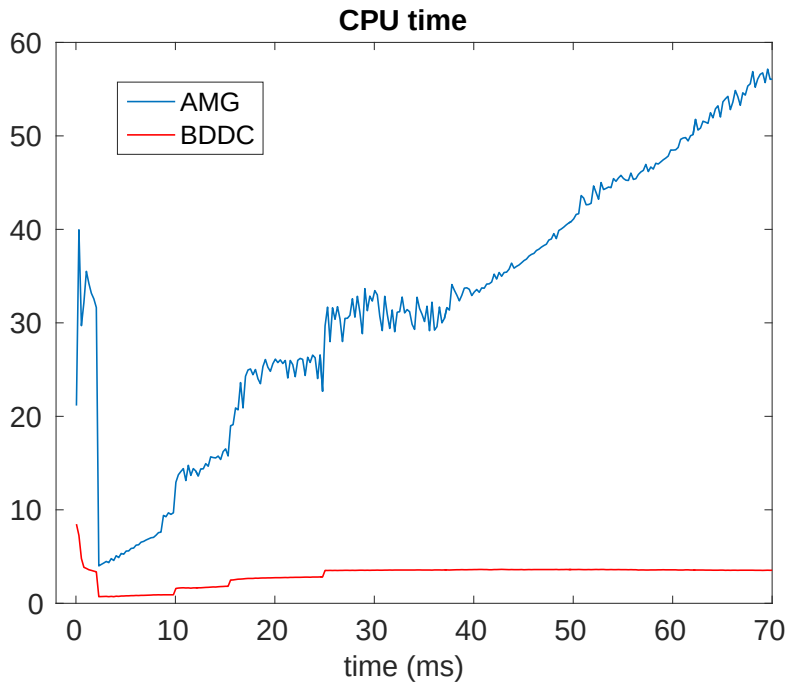
Robustness of mechanical solver with respect to deformation: Newton iterations



Robustness of mechanical solver with respect to deformation: GMRES iterations

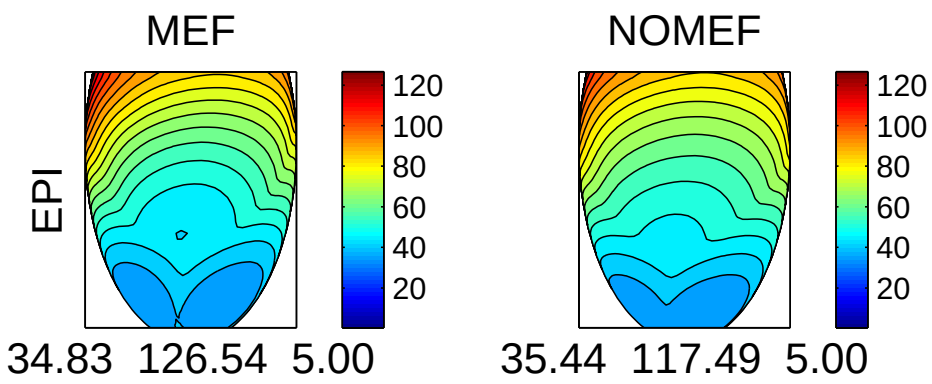


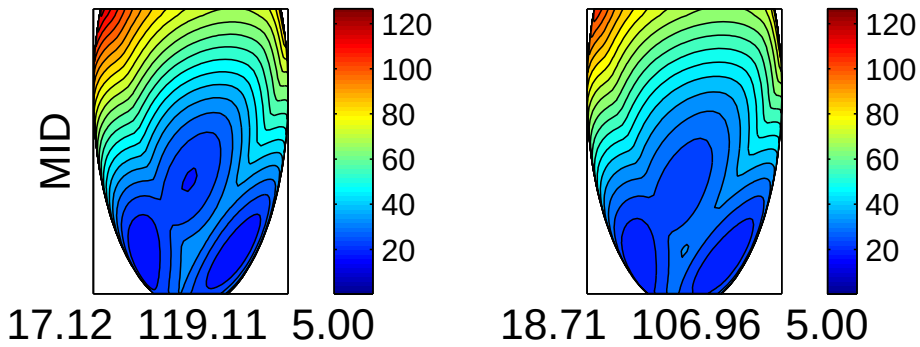
Robustness of mechanical solver with respect to deformation: CPU time

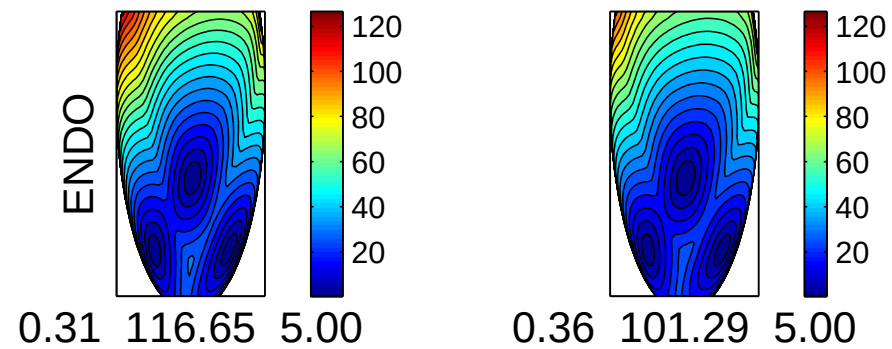


Effects of MEFs on the activation sequence

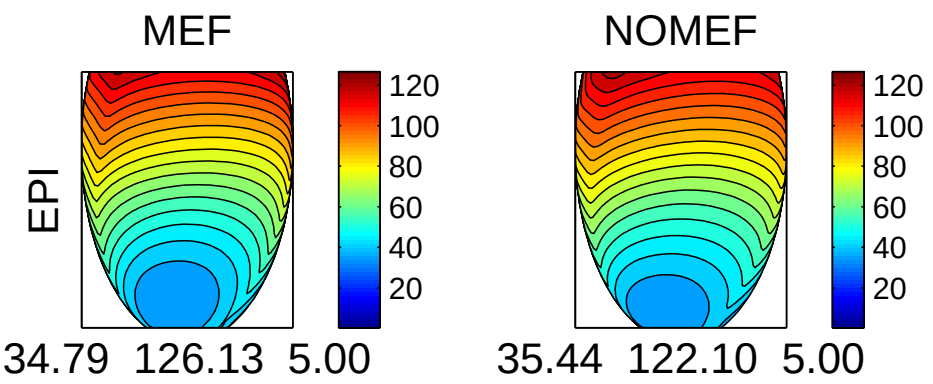
Anterior View

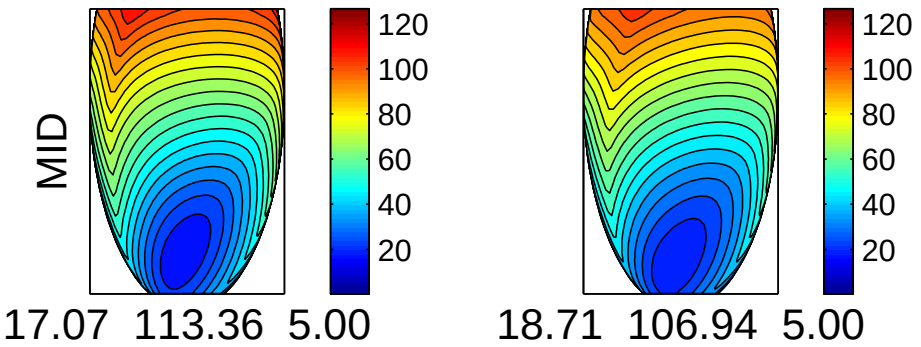


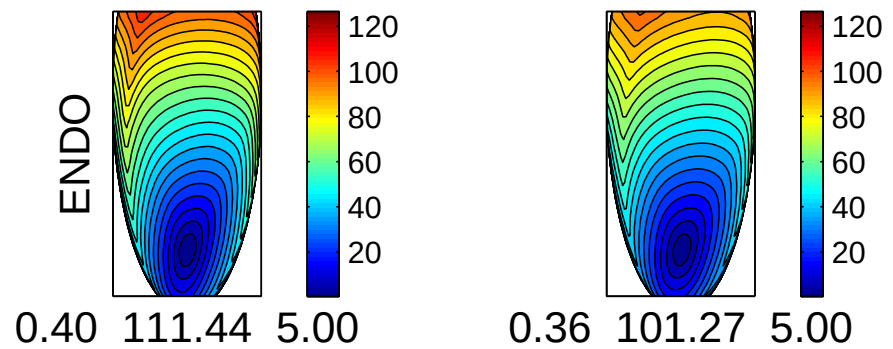




Posterior View

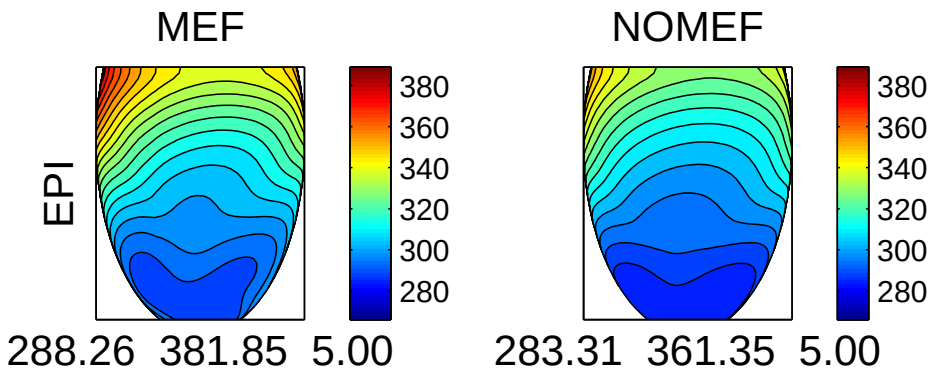




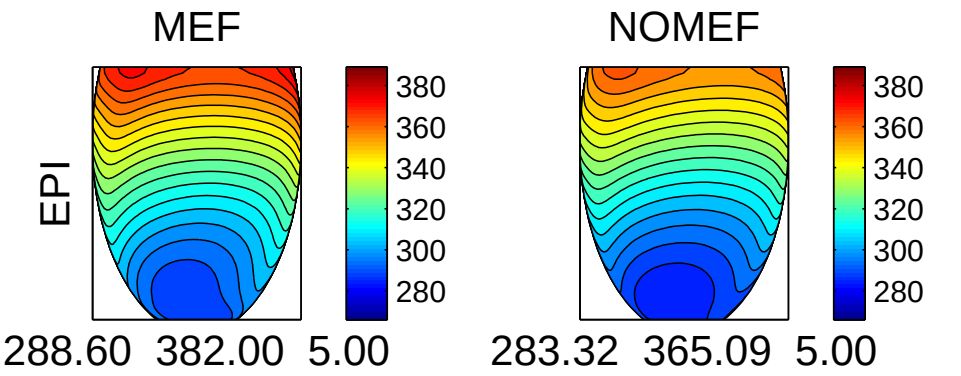


Effects of MEFs on the repolarization sequence

Anterior View

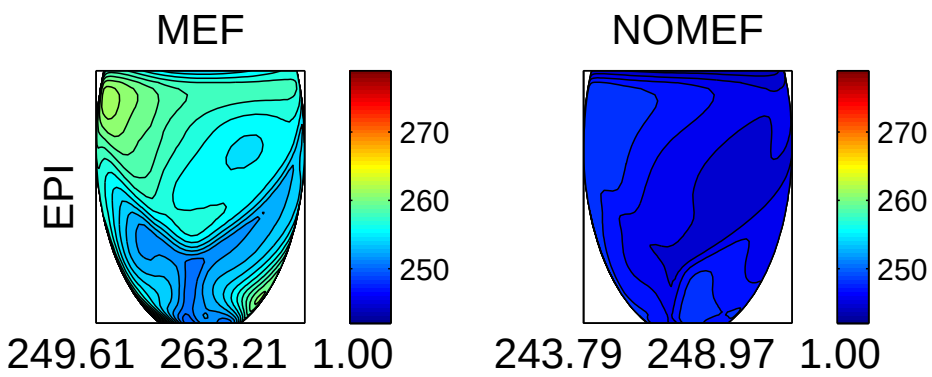


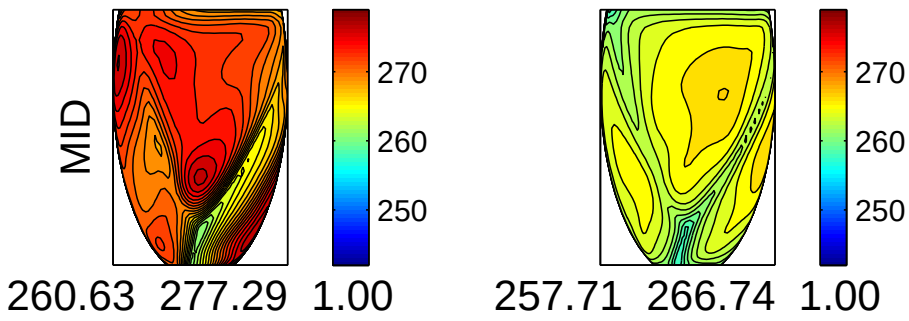
Posterior View

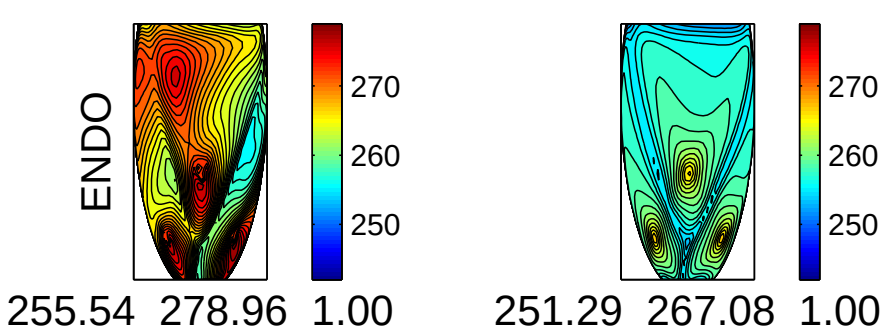


Effects of MEFs on the action pot. duration(APD)

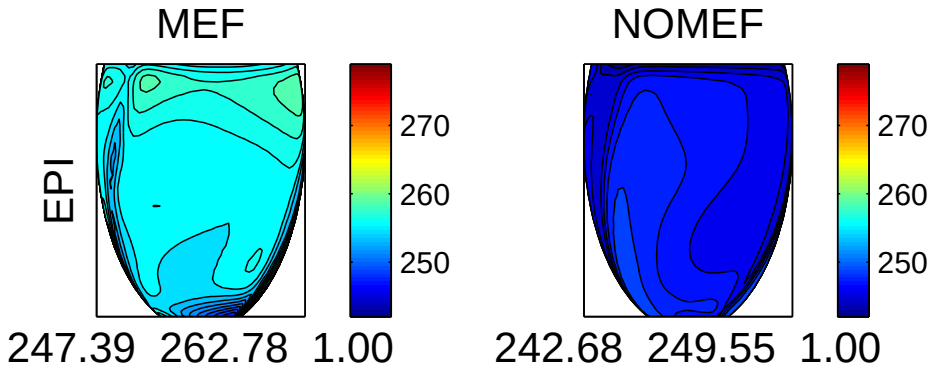
Anterior View

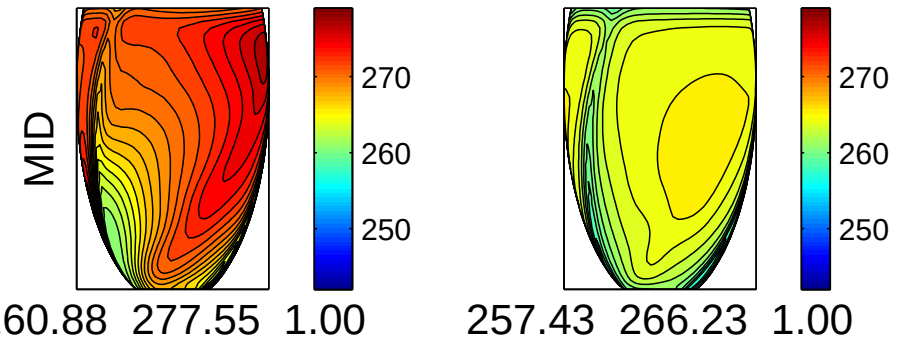


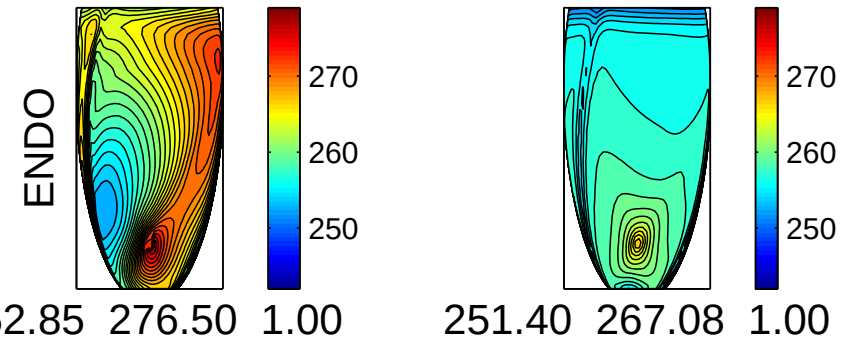




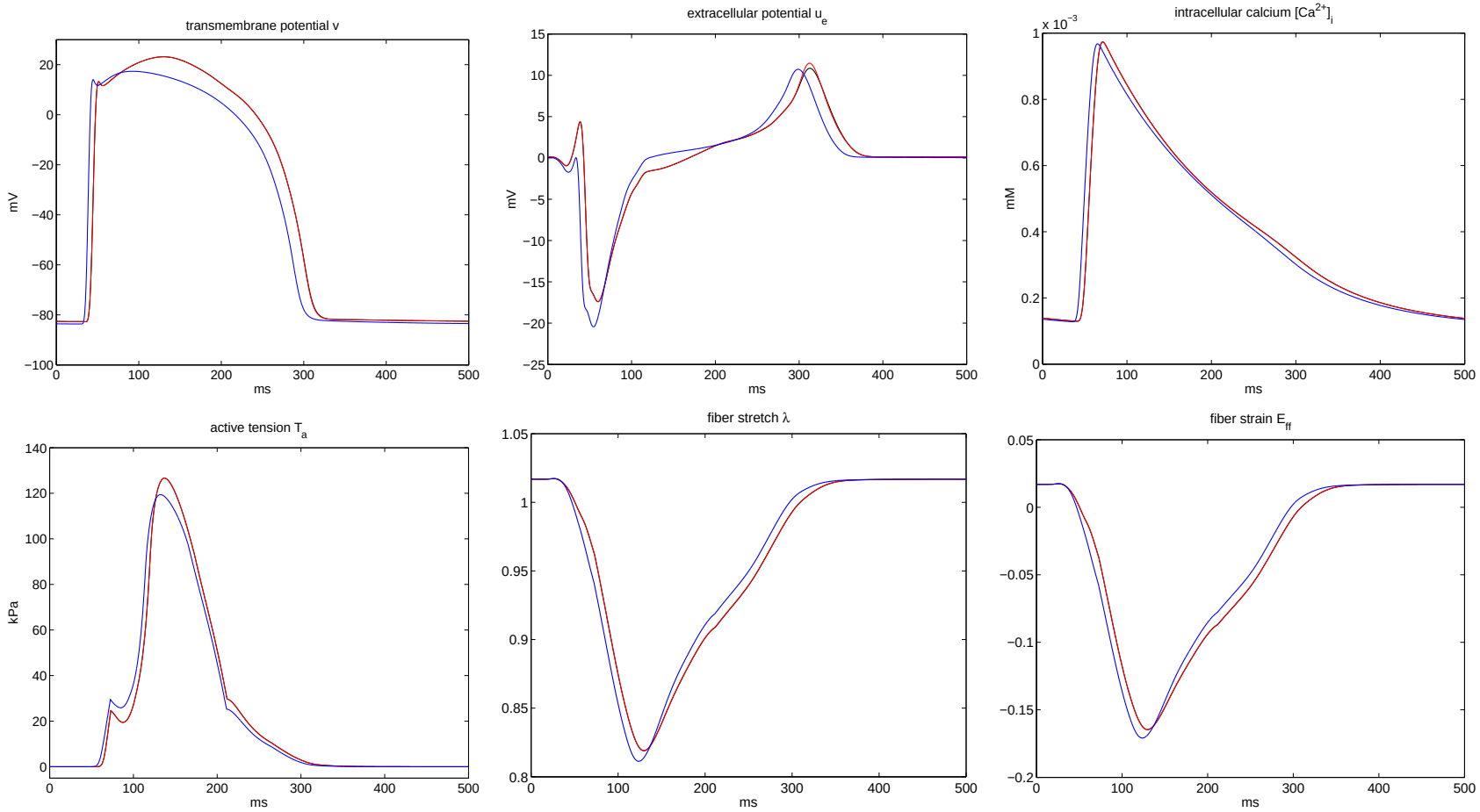
Posterior View







Waveforms. **AP:** v - **EG:** u_e - Ca_i – Ta – λ – E_{ff}



Conclusions

Developed a scalable solver for the cardiac electromechanical coupling, based on Multilevel Additive Schwarz and BDDC preconditioners

Further work should be devoted to the construction of

- Multivel BDDC preconditioners,
- BDDC preconditioners with minimal coarse space,
- BDDC preconditioners for mixed discretizations of the mechanical system.

THANK YOU