Multilevel Schwarz and Multigrid preconditioners for the Bidomain system

S. Scacchi
Università di Pavia

Joint work with L. Pavarino
Università di Milano

17th International Conference on Domain Decomposition Methods
St. Wolfgang/Strobl, Austria, July 3-7 2006

Outline

- 1. Introduction to the Bidomain model
- 2. Numerical methods
- 3. Parallel implementation
- 4. Numerical results

The macroscopic Bidomain model

Reaction-Diffusion system of two parabolic PDEs coupled with a system of ODEs.

DATA: $I_{app}^{i,e}$ (applied current per unite volume), v_0, w_0, c_0 (initial conditions)

UNKNOWNS: u_i, u_e (intra and extracellular potentials), w (gating variables), c (ion concentrations)

$$\begin{cases} \rho C_m \frac{\partial v}{\partial t} - div(D_i \nabla u_i) + \rho I_{ion}(v, w, c) = I_{app}^i & \text{in } \Omega \times (0, T) \\ -\rho C_m \frac{\partial v}{\partial t} - div(D_e \nabla u_e) - \rho I_{ion}(v, w, c) = I_{app}^e & \text{in } \Omega \times (0, T) \\ \frac{\partial w}{\partial t} = R(v, w), \quad \frac{\partial c}{\partial t} = S(v, w, c) & \text{in } \Omega \times (0, T) \end{cases}$$

+ 0 Neumann b.c. for u_i, u_e and initial conditions for v, w, c.

$v = u_i - u_e =$ transmembrane potential, ρ ratio of membrane area/tissue volume, C_m surface capacitance, $I_{ion}(v, w, c)$ is the ionic current resulting from membrane model, $D_{i,e}$ are the intra and extracellular conductivity tensors

Membrane models

- System of ODEs for gating and ion concentrations variables that model the ionic exchanges through the cellular membrane
- First membrane model proposed by Hodgkin and Huxley in '50
- Membrane models for Left Ventricle: Beeler-Reuter(1977), Luo-Rudy I(1991), Luo-Rudy II(1994),...

Finite element discretization in space

- Portion of Left Ventricle is modeled with a slab
- Structured grid, trilinear finite elements

$$V_h = \{\varphi_h \text{ continuous in } \Omega \text{ and } \varphi_{h|K} \in Q_1,\ \forall K \in \tau_h\}$$

- Bidomain semidiscrete system

$$\begin{cases} \rho C_m \mathcal{M} \frac{\partial}{\partial t} \begin{pmatrix} u_{i,h} \\ u_{e,h} \end{pmatrix} + \mathcal{A} \begin{pmatrix} u_{i,h} \\ u_{e,h} \end{pmatrix} + \rho \begin{pmatrix} MI^h_{ion} \\ -MI^h_{ion} \end{pmatrix} = \begin{pmatrix} MI^{i,h}_{app} \\ -MI^{e,h}_{app} \end{pmatrix} \\ \frac{\partial w_h}{\partial t} = R(v_h, w_h), \quad \frac{\partial c_h}{\partial t} = S(v_h, w_h, c_h) \end{cases}$$

where

$$\mathcal{M} = \begin{bmatrix} M & -M \\ -M & M \end{bmatrix}, \qquad \mathcal{A} = \begin{bmatrix} A_i & 0 \\ 0 & A_e \end{bmatrix}$$

Time discretization: semi-implicit method (IMEX)

- implicit treatment of the gating variables w
- explicit treatment of the ionic concentrations variables c
- implicit treatment of the linear diffusion term
- explicit treatment of the nonlinear reaction term
- Adaptive time-step strategy based on $\Delta v = max(v^n - v^{n-1})$:
  if $\Delta v < \Delta v_{min} = 0.05$ then $\Delta t = (\frac{\Delta v_{max}}{\Delta v})\Delta t$
  if $\Delta v > \Delta v_{max} = 0.5$ then $\Delta t = (\frac{\Delta v_{min}}{\Delta v})\Delta t$
  $\Delta t_{min} = 0.005 msec < \Delta t < \Delta t_{max} = 6 msec$

Time discretization II

Given $\mathbf{v}^n = \mathbf{u}_i^n - \mathbf{u}_e^n$, $\mathbf{w}^n$, $\mathbf{c}^n$,

Find $\mathbf{w}^{n+1}$, $\mathbf{c}^{n+1}$ by

$$\frac{\mathbf{w}^{n+1} - \mathbf{w}^n}{\Delta t} = R(\mathbf{v}^n, \mathbf{w}^{n+1}, \mathbf{c}^n), \qquad \frac{\mathbf{c}^{n+1} - \mathbf{c}^n}{\Delta t} = S(\mathbf{v}^n, \mathbf{w}^{n+1}, \mathbf{c}^n)$$

and then $\mathbf{u}_i^{n+1}$, $\mathbf{u}_e^{n+1}$ solving the linear system

$$\left(\frac{\rho C_m}{\Delta t}\mathcal{M} + \mathcal{A}\right)\begin{pmatrix} \mathbf{u}_{i,h}^{n+1} \\ \mathbf{u}_{e,h}^{n+1} \end{pmatrix} =$$

$$-\rho\begin{pmatrix} MI_{ion}^h(\mathbf{v}^n, \mathbf{w}^{n+1}, \mathbf{c}^{n+1}) \\ -MI_{ion}^h(\mathbf{v}^n, \mathbf{w}^{n+1}, \mathbf{c}^{n+1}) \end{pmatrix} + \mathcal{M}\begin{pmatrix} \mathbf{u}_{i,h}^n \\ \mathbf{u}_{e,h}^n \end{pmatrix} + \begin{pmatrix} MI_{app}^{i,h} \\ -MI_{app}^{e,h} \end{pmatrix}$$

The choice of preconditioners

- At each time step we have to solve a linear system with iteration matrix
$$(\frac{\rho C_m}{\Delta t}\mathcal{M} + \mathcal{A})$$
which is singular and very ill-conditioned
- One level preconditioners (Block Jacobi, One level Schwarz) are not scalable
- The simulation of a whole heartbeat in a portion of ventricle (4×10^6 d.o.f.) with 36 processors of a Linux cluster (2.8 GH) takes about 50 hours
- Need multilevel preconditioners

Multigrid preconditioner

- Firstly used by Dos Santos for Bidomain in elliptic case (IEEE Trans. Biomed. Eng. 2004)
- V-cycle multigrid method
- Block-Jacobi smoother
- For the coarsest grid we use the parallel PCG (toll=10^{-8}) preconditioned by BJ

Symmetrized Multiplicative Multilevel Schwarz Preconditioner (SMMS)

See e.g. Dryja, Widlund (Proc. Sixth GAMM-Sem. 1991) and Zhang (Num. Math. 1992).
Let be

- $\Omega^{(i)}$ $i = 0, ..., M$ family of triangulations of Ω
- $A^{(i)}$ the matrices obtained discretizing the PDEs on $\Omega^{(i)}$
- $R^{(i)}$ the restriction operator from $\Omega^{(i+1)}$ to $\Omega^{(i)}$

Decompose $\Omega^{(i)}$ in $N^{(i)}$ overlapping subdomains and consider

- $R_k^{(i)} : \Omega^{(i)} \longrightarrow \Omega_k^{(i)}$ the restriction operator for the domain $\Omega_k^{(i)}$
- $A_k^{(i)} = R_k^{(i)} A^{(i)} R_k^{(i)^T}$ the subblock of $A^{(i)}$ associated with domain $\Omega_k^{(i)}$

SMMS-The algorithm I

$$u^{(M)} \leftarrow \sum_{k=1}^{N^{(M)}} R_k^{(M)^T} A_k^{(M)^{-1}} R_k^{(M)} r$$

$$r^{(M-1)} \leftarrow R^{(M-1)} \left(r - A^{(M)} u^{(M)} \right)$$

$$u^{(M-1)} \leftarrow \sum_{k=1}^{N^{(M-1)}} R_k^{(M-1)^T} A_k^{(M-1)^{-1}} R_k^{(M-1)} r^{(M-1)}$$

$$r^{(M-2)} \leftarrow R^{(M-2)} \left(r^{(M-1)} - A^{(M-1)} u^{(M-1)} \right)$$

$$\dots$$

$$u^{(0)} \leftarrow A^{(0)^{-1}} r^{(0)}$$

SMMS-The algorithm II

$$u^{(1)} \leftarrow u^{(1)} + R^{(0)^T} u^{(0)}$$

$$u^{(1)} \leftarrow u^{(1)} + \sum_{k=1}^{N^{(1)}} R_k^{(1)^T} A_k^{(1)^{-1}} R_k^{(1)} (r^{(1)} - A^{(1)} u^{(1)})$$

$$\dots$$

$$u^{(M)} \leftarrow u^{(M)} + R^{(M-1)^T} u^{(M-1)}$$

$$u^{(M)} \leftarrow u^{(M)} + \sum_{k=1}^{N^{(M)}} R_k^{(M)^T} A_k^{(M)^{-1}} R_k^{(M)} (r^{(M)} - A^{(M)} u^{(M)})$$

$$u \leftarrow u^{(M)}$$

SMMS-Remarks

Remarks on the algorithm

- Additive in levels: the local problems can be solved in parallel
- Multiplicative between levels: sequential through the levels

Remarks on the implementation

- For local problems we use ILU(0) solver
- For the coarsest grid we use the parallel PCG (toll=10^{-8}) preconditioned by BJ

Parallel implementation

- Code written in FORTRAN 90
- Parallel solver is based on:
  parallel library PETSc from Argonne National Laboratory
  preconditioned Krylov subspace methods (KSP and PC PETSc object)
- Platforms:
  IBM Linux Cluster of University of Milan (72 CPU, 2.4 GHz, 1 Gb every 2 CPU)
  IBM Linux Cluster CLX of CINECA(1024 CPU, 3 GHz, 1 Gb every 2 CPU)

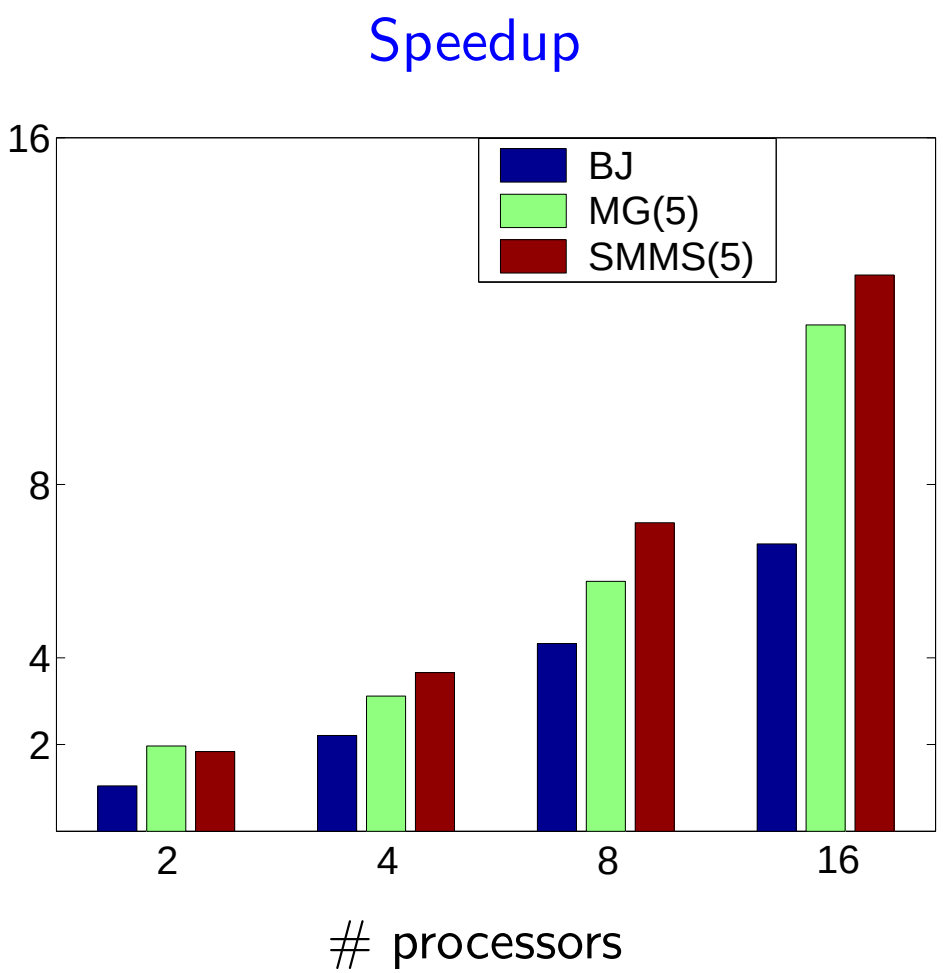
Test 1: Fixed global load

- Simulate 0.5 ms (10 time steps) of ventricle excitation
- Domain is a $2.56 \times 2.56 \times 0.01 cm^3$ slab discretized by a $256 \times 256 \times 2$ finite elements grid (262144 d.o.f.)
- Run on Linux cluster of University of Milan

Test 1

# SUB	BJ		MG(5)		SMMS(5)	
	IT.	TIME	IT.	TIME	IT.	TIME
1	95	23.00	3	9.11	-	-
2	108	22.27	3	4.63	3	4.95
4	109	10.40	4	2.92	3	2.49
8	111	5.31	4	1.58	3	1.28
16	114	3.47	4	0.78	3	0.71

Test 1



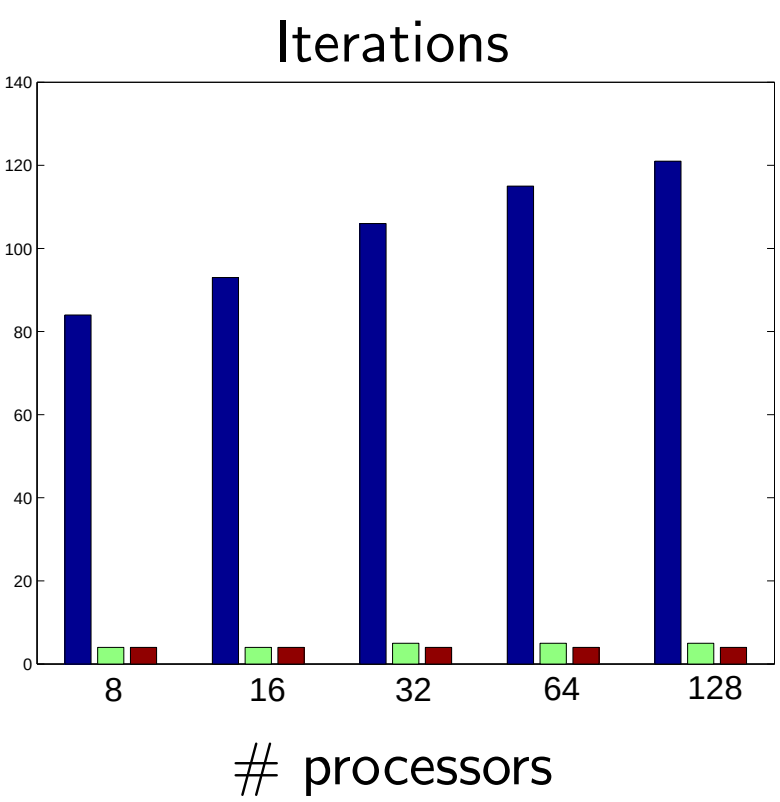
Test 2: Fixed local load

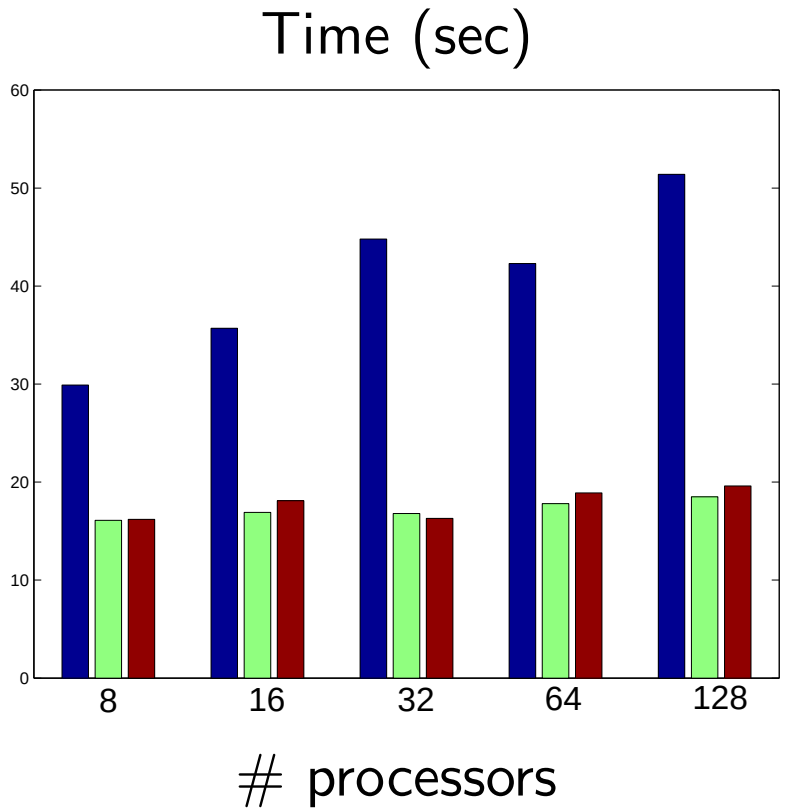
- Simulate 0.5 ms (10 time steps) of ventricle excitation
- Fixed Subdomain mesh $48 \times 48 \times 48$, i.e. 221184 d.o.f.
- Run on CLX cluster of CINECA

Test 2

# SUB	D.O.F.	BJ		MG(5)		SMMS(5)	
		IT.	TIME	IT.	TIME	IT.	TIME
8	1769472	84	29.9	4	16.1	4	16.2
16	3538944	93	35.7	4	16.9	4	18.1
32	7077888	106	44.8	5	16.8	4	16.3
64	14155776	115	42.3	5	17.8	4	18.9
128	28311552	121	51.4	5	18.5	4	19.6

Test 2


Iterations
140
120
100
80
60
40
20
0
8
16
32
64
128
processors


Time (sec)
60
50
40
30
20
10
0
8
16
32
64
128
processors

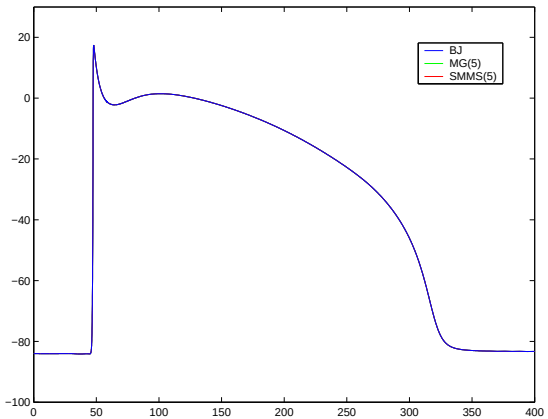
Test 3: Complete Heartbeat

- Simulate a complete heartbeat (400 ms, i.e. about 3000 time steps) in a portion of ventricle having dimensions $2 \times 2 \times 0.5\, cm^3$
- Mesh size $= 200 \times 200 \times 50$, 4000000 d.o.f.
- 36 subdomains
- Run on Linux cluster of University of Milan

Test 3

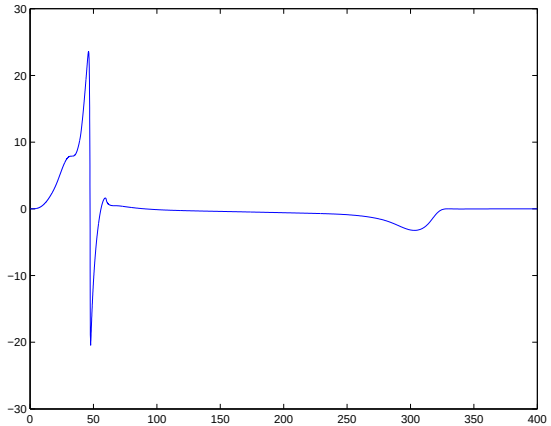
PREC	IT. (AVER.)	TIME (AVER.)	TOTAL TIME
BJ	205	46.02 sec	29 h 49 m
MG(5)	8	11.11 sec	7 h 21 m
SMMS(5)	6	9.67 sec	6 h 26 m

Transmembrane potential



time (ms)

Extracellular potential

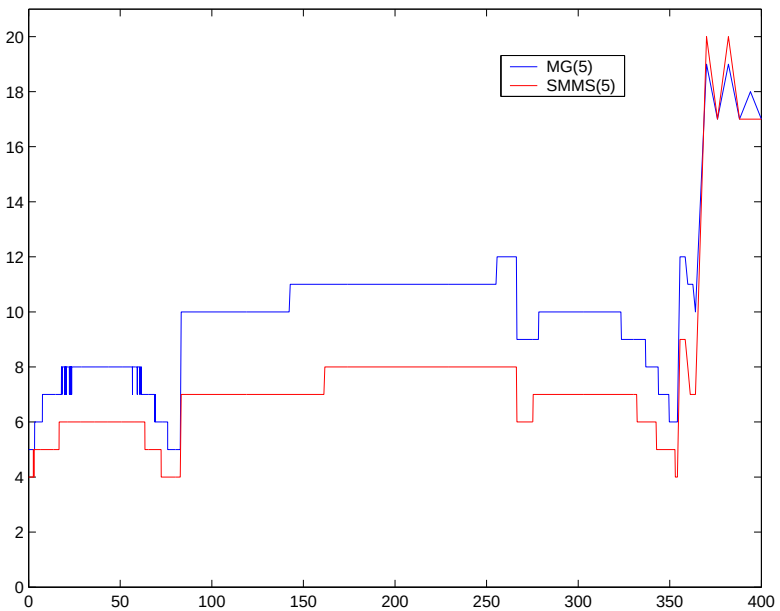


time (ms)

Test 3

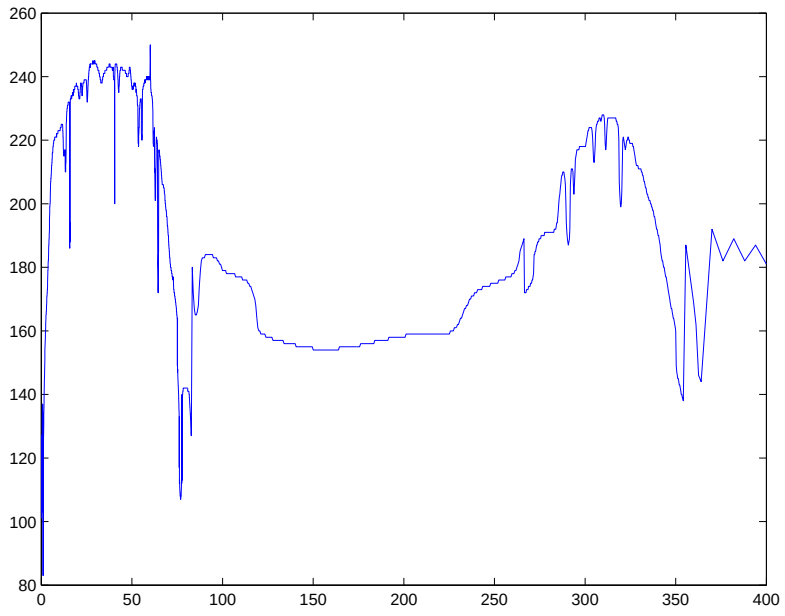
Time evolution of the PCG iterations

MG(5)-SMMS(5)



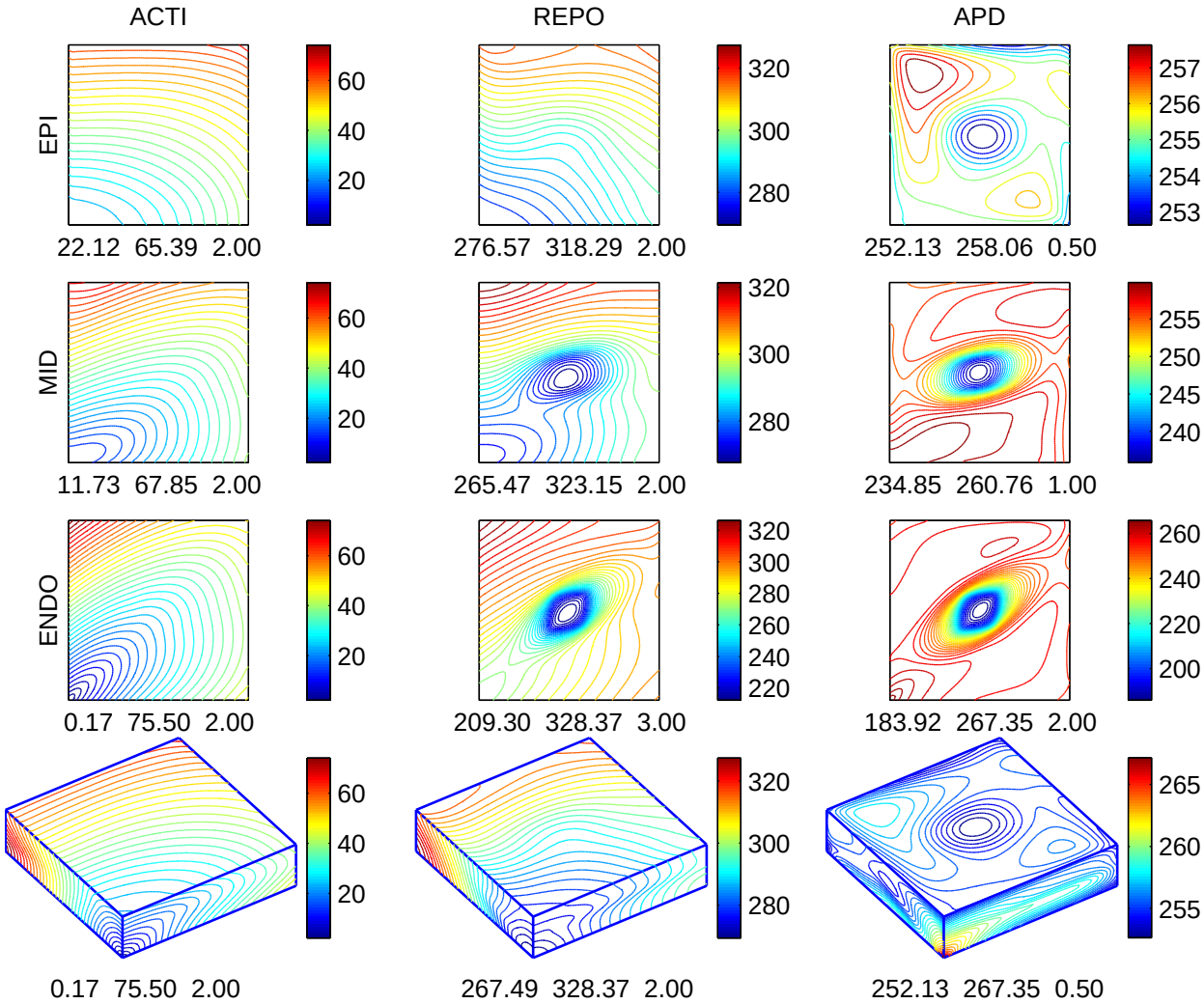
time (ms)

Block Jacobi



time (ms)

Test 3: Activation and Repolarization times



Conclusions and developments

- MG and SMMS preconditioners are optimal for the Bidomain system: scalable and efficient
- The complete heartbeat simulation time is reduced four times compared with BJ
- Extend to more realistic domains (ellipsoidal)
- Extend to unstructured meshes
- Consider the presence of arrhythmias