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SPPEXA

Time Parallel and Space –Time Approaches in Electrophysiology

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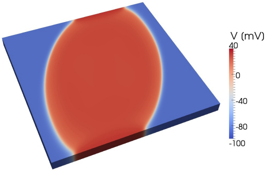
Computational electrocardiology

- Simulation of the electrical activation sequence of the human heart
- Modeled by FitzHugh-Nagumo equation: nonlinear reaction diffusion:

$$\partial_t V - \nabla \cdot (\mathbf{D}(\mathbf{x}) \nabla V) = I_{ion}(V) + I_{ext} \qquad in\ \Omega \times [0, T],$$

$V(\mathbf{x}, t) :=$ electric potential
$\mathbf{D(x)} :=$ conductivity tensor
$I_{ion}(V) = V \cdot (a - V)(V - 1) \quad$ with $\quad 0 < a < 1$
$I_{ext} :=$ external current



Challenges

- Requires high local spatial and temporal resolution to capture wave front.
- Multiscale structure in space and time.
  - Space scale: from 0.1 mm to centimeters
  - Time scale : from 0.1 msec to ~ 1 second for
- Realistic 3D simulations need $\sim O(10^7)$ unknowns.

$$\Downarrow$$

Parallel solver in space AND time!

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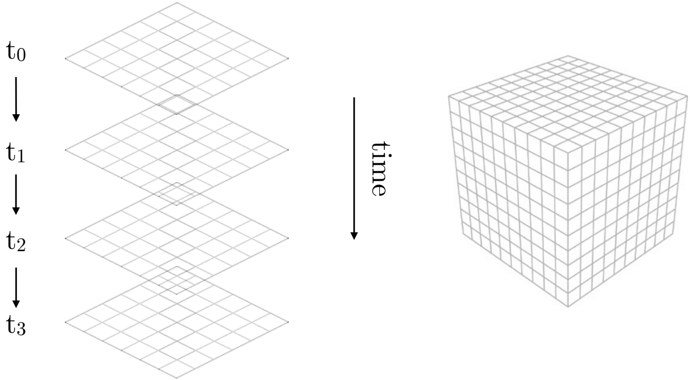
Why space–time for parallel in time?

Time stepper vs space–time discretization (2D+1):



Memory issues? Not really...

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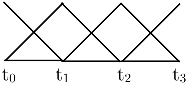
- Continuous finite element (CG) in space
- Discontinuous finite element (DG) in time[1] $\longrightarrow$ Why?

CG

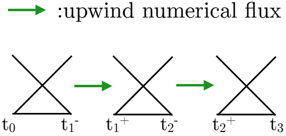


p+1

✗ need stabilization

✓ easier to implement

DG



✓ 2p+1

✓ A-stable

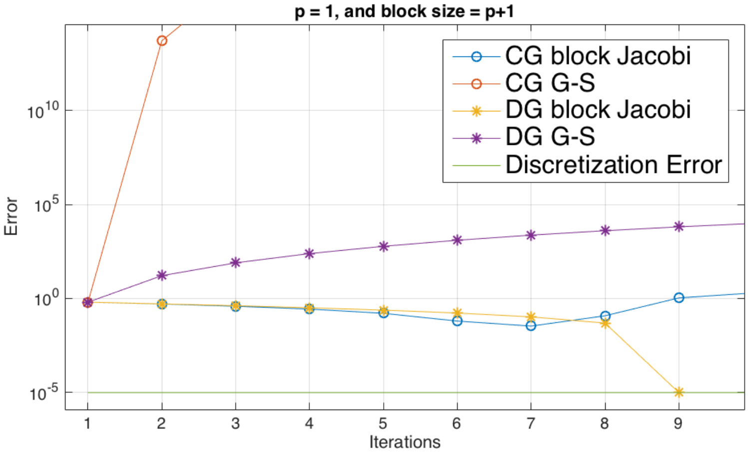
✓ block structure

✗ more DoFs (?)

[1] Lasaint and Raviart: "On a finite element method for solving the neutron transport equation", 1974

CG vs DG tests for smoothing

Dahlquist test ODE for smoothers:



Space-time Assembling[2]

Let's consider, to simplify notation, heat equation with a possibly non linear right hand side $f = f(\mathbf{x}, t)$

$$\partial_t V - \nabla \cdot (\mathbf{D}(\mathbf{x}) \nabla V) = f$$

- Divide the time interval $[0, T]$ in time 'slabs'

$$0 = t_0 < t_1 < \ldots < t_m < t_m + 1 < \ldots < t_N = T$$

- Weak formulation on the time slab $\mathscr{E}^m = [t_m, t_{m+1}] \times \Omega$ for test function $U \in C^1(\mathscr{E}^m)$ vanishing on $\partial\Omega$

$$\int_{\mathscr{E}^m} \partial_t V \, U \, \mathrm{d}t\mathrm{d}\mathbf{x} - \int_{\mathscr{E}^m} \nabla \cdot (\mathbf{D}(\mathbf{x}) \nabla V) \, U \, \mathrm{d}t\mathrm{d}\mathbf{x} = \int_{\mathscr{E}^m} f \, U \, \mathrm{d}t\mathrm{d}\mathbf{x}$$

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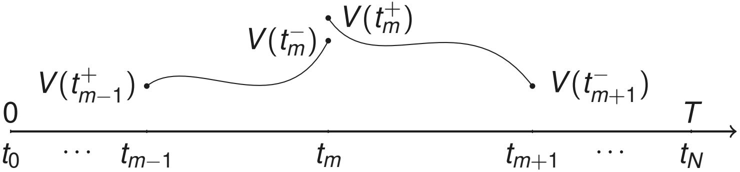
[2] Jamet. "Galerkin-type approximations which are discontinuous in time for parabolic equations in a variable domain", 1978.

$$\underline{\int_{\mathcal{E}^m} \partial_t V\, U \,\mathrm{d}t\mathrm{d}\mathbf{x}} - \int_{\mathcal{E}^m} \nabla \cdot (\mathbf{D} \nabla V)\, U \,\mathrm{d}t\mathrm{d}\mathbf{x} = \int_{\mathcal{E}^m} f\, U \,\mathrm{d}t\mathrm{d}\mathbf{x}$$

- integration by parts

$$\underline{-\int_{\mathcal{E}^m} V\, \partial_t U \,\mathrm{d}t\mathrm{d}\mathbf{x} + \int_{\Omega} \left[V\, U\right]_{t_m}^{t_{m+1}} \mathrm{d}\mathbf{x}} + \int_{\mathcal{E}^m} \mathbf{D} \nabla V\, \nabla U \,\mathrm{d}t\mathrm{d}\mathbf{x} = \int_{\mathcal{E}^m} f\, U \,\mathrm{d}t\mathrm{d}\mathbf{x}$$



- Upwind numerical flux on V

$$\left[V\, U\right]_{t_m}^{t_{m+1}} := V(t_{m+1}^-)U(t_{m+1}^-) - V(t^{-}{}_{m})U({}^{+}t_m)$$

$$\underline{-\int_{\mathscr{E}^m} V\,\partial_t U\,\mathrm{d}t\mathrm{d}\mathbf{x}} + \underline{\int_\Omega \left[V\,U\right]_{t_m}^{t_{m+1}}\mathrm{d}\mathbf{x}} + \underline{\int_{\mathscr{E}^m}\mathbf{D}\nabla V\,\nabla U\,\mathrm{d}t\mathrm{d}\mathbf{x}} = \int_{\mathscr{E}^m} f\,U\,\mathrm{d}t\mathrm{d}\mathbf{x}$$

- We choose function space in a tensor form

$$V_h^m(\mathbf{x},t) = \sum_l \sum_k v_{l,k}^m \psi_l(\mathbf{x})\phi_k(t)$$

- We can now separate variables, for the i,j contribution of the left hand side we get:

$$\underline{-\int_{t_m}^{t_{m+1}} \phi_j(t)\phi_i'(t)\mathrm{d}t \int_\Omega \psi_j(\mathbf{x})\psi_i(\mathbf{x})\mathrm{d}\mathbf{x}}$$

$$\underline{+\left[\phi_j(t_{m+1}^-)\phi_i(t_{m+1}^-) - \phi_j(t_m^-)\phi_i(t_m^+)\right]\int_\Omega \psi_j(\mathbf{x})\psi_i(\mathbf{x})\mathrm{d}\mathbf{x}}$$

$$\underline{+\int_{t_m}^{t_{m+1}} \phi_j(t)\phi_i(t)\mathrm{d}t \int_\Omega \mathbf{D}\nabla\psi_j(\mathbf{x})\cdot\nabla\psi_i(\mathbf{x})\mathrm{d}\mathbf{x}.}$$

Time and Space operators[3]:

$$\underline{\left[\phi_j(t_{m+1}^-)\phi_i(t_{m+1}^-) - \int_{t_m}^{t_{m+1}} \phi_j(t)\phi_i'(t)\mathrm{d}t\right]}\,\underline{\int_\Omega \psi_j(\mathbf{x})\psi_i(\mathbf{x})\mathrm{d}\mathbf{x}} \longrightarrow K_t \otimes M_h$$

$$\underline{\phi_j(t_m^-)\phi_i(t_m^+)}\,\underline{\int_\Omega \psi_j(\mathbf{x})\psi_i(\mathbf{x})\mathrm{d}\mathbf{x}} \longrightarrow N_t \otimes M_h$$

$$\underline{\int_{t_m}^{t_{m+1}} \phi_j(t)\phi_i(t)\mathrm{d}t}\,\underline{\int_\Omega \nabla\psi_j(\mathbf{x})\cdot\nabla\psi_i(\mathbf{x})\mathrm{d}\mathbf{x}} \longrightarrow M_t \otimes K_h$$

$$A = K_t \otimes M_h + M_t \otimes K_h$$

$$B = N_t \otimes M_h$$

$$\begin{bmatrix} A & & & \\ B & A & & \\ & \ddots & \ddots & \\ & & B & A \end{bmatrix} \begin{bmatrix} \mathbf{u}_{t_1} \\ \mathbf{u}_{t_2} \\ \vdots \\ \mathbf{u}_{t_N} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{t_1} \\ \mathbf{f}_{t_2} \\ \vdots \\ \mathbf{f}_{t_N} \end{bmatrix}$$

[3] Gander and Neumüller: “Analysis of a new space-time parallel multigrid algorithm for parabolic problems”, 2016.

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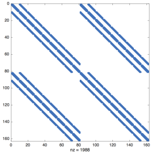
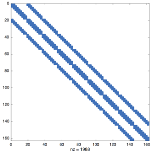
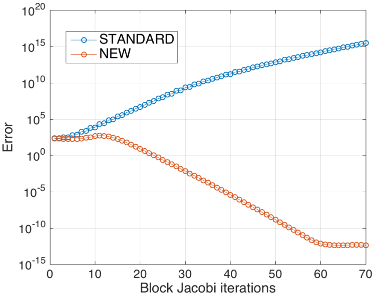
Space–Time vs Time–Space

- Ordering of basis function is arbitrary but...

$$M_t \otimes M_h \neq M_h \otimes M_t$$

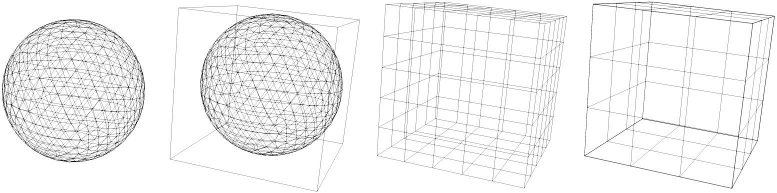






Space–Time Semi–Geometric Multigrid

- We developed a multigrid solver for the space–time system[4]
  - Parallel assembly and solution (block Jacobi)
  - Flexible for selection coarsening strategies
- Coarsening strategy
  - Input vector example for 4 levels: $[ST, T, ST, S]$
  - Spatial coarsening: L^2 Volume Projection for space coarsening[5]

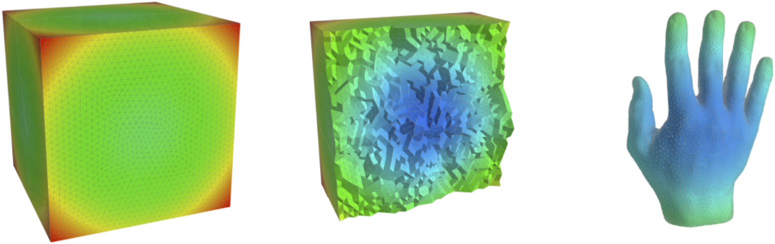


  - Time coarsening: 1D bisection.

[4] Horton and Vandewalle: “A space-time multigrid method for parabolic partial differential equations” , 1995

[5] Krause and Zulian: “A Parallel Approach to the Variational Transfer of Discrete Fields between Arbitrarily Distributed Unstructured Finite Element Meshes”, 2015

Transfer the data from a **source** mesh to a **target** mesh



(a) Source mesh. (b) Source mesh cut. (c) Target mesh.

$\Omega_s, \Omega_t \subset \mathbb{R}^d$: bounded domains approximated by Ω_s^h and Ω_t^h,

$\mathscr{M}_s$ and $\mathscr{M}_t \to$ associated meshes

$V_h = V_h(\mathscr{M}_s)$ and $W_h = W_h(\mathscr{M}_t) \to$ associated spaces.

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L^2 Volume Projection for space coarsening

- Define a suitable discrete space of test functions M_h
- Set M_h as a **discrete space** based on **the same space as the target mesh**

L^2 Projection definition: weak form

$$\int_{I_h} (v_h - P(v_h))\mu_h \, d\mathbf{x} = \int_{I_h} (v_h - w_h)\mu_h \, d\mathbf{x} = 0 \quad \forall \mu_h \in M_h$$

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$$\Downarrow$$

$$\sum_{i \in J_v} v_i \int_{I_h} \phi_i \psi_k \, d\mathbf{x} = \sum_{j \in J_w} w_j \int_{I_h} \theta_j \psi_k \, d\mathbf{x} \qquad \text{for } k \in J_\mu .$$

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$$\Downarrow$$

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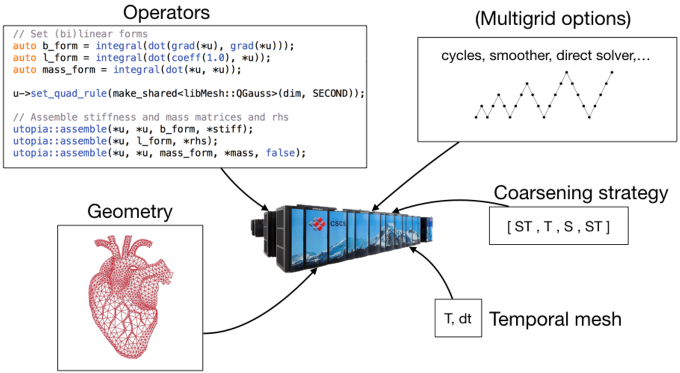
$$\Downarrow$$

$$\mathbf{w} = \mathbf{D}^{-1}\mathbf{B}\mathbf{v} = \mathbf{T}\mathbf{v}$$

Implementation

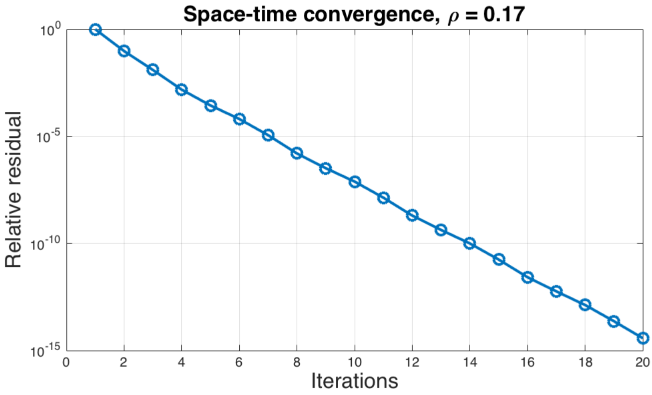
- UTOPIA[6]
  - C++ embedded domain specific language designed for parallel non-linear solution strategies and finite element analysis
- PETSc and libMesh backends



[6] Zulian, Schneider, Kopanicakova, Krause: “Utopia: A C++ Embbeded Domain Specific Language for Scientific Computing”, 2017.

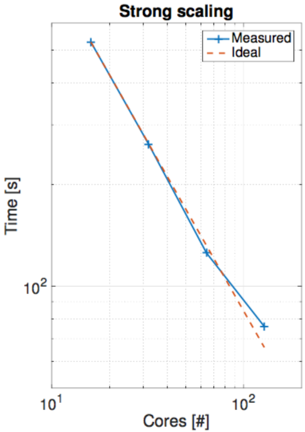
Heat equation - MG convergence

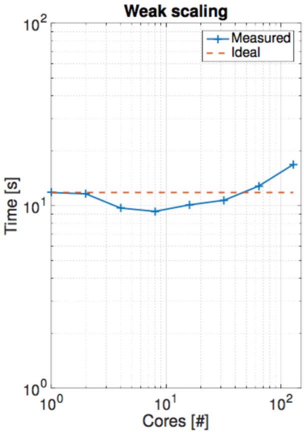
- Parallel block Jacobi smoothing
- Gauss-Seidel inside the block
- The block choice is line smoothing in time
- Space-time coarsening



Heat equation - Scaling

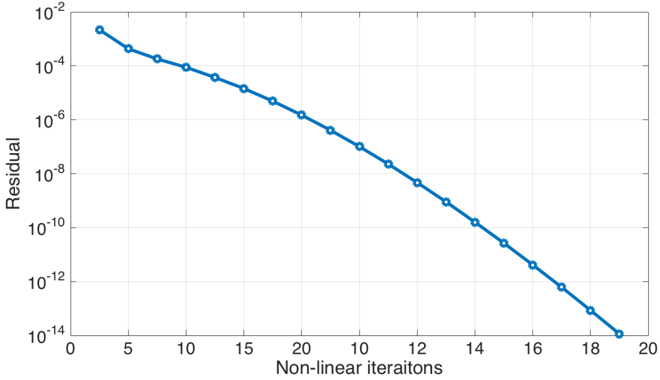
$\approx 2 \cdot 10^6$ DoFs





FitzHugh-Nagumo: $\partial_t V - D\Delta V = I_{ion}(V)$

- Non-linearity is treated explicitly
- **Problem**: in a realistic setting D is very small!
- **Idea**: Initially use just space coarsening. Example:
  - Space–time coarsening diverges!
  - Space coarsening + ST coarsening:



Space-time Spectral Analysis[7]

We performed a spectral analysis of the heat equation with diffusion coefficient $K(\mathbf{x})$ and homogeneous Dirichlet initial/boundary conditions

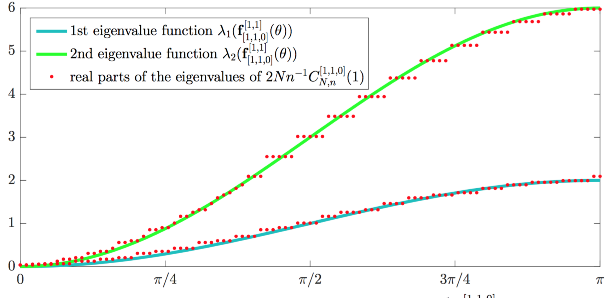
$$\begin{cases} \partial_t u - \nabla \cdot K(\mathbf{x})\nabla u = f \\ u(\mathbf{x},0) = u_0 \end{cases}$$

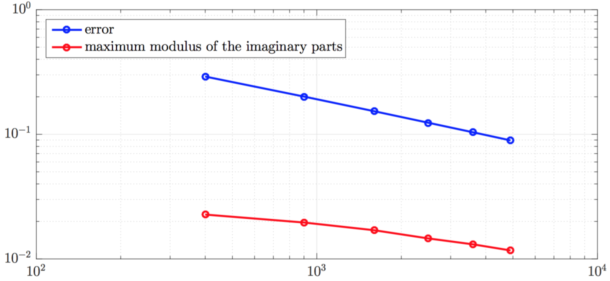
Discretized in space-time with DG in time and finite element in space (with arbitrary regularity)

$$\begin{bmatrix} A & & & \\ B & A & & \\ & \ddots & \ddots & \\ & & B & A \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_N \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_N \end{bmatrix} \iff C_n \mathbf{u}_n = \mathbf{f}_n$$

[7] Benedusi, Garoni, Li, Krause, Serra-Capizzano: ”Space-Time FE-DG Discretization of the Anisotropic Diffusion Equation in any Dimension: the Spectral Symbol”

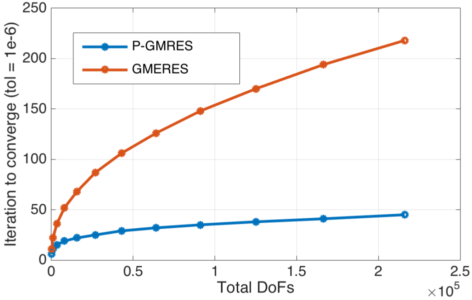
Space-time Spectral Analysis: Numerical Experiments





$$C = \begin{bmatrix} A & & & \\ B & A & & \\ & \ddots & \ddots & \\ & & B & A \end{bmatrix}, \qquad P = \begin{bmatrix} A_p & & & \\ & A_p & & \\ & & \ddots & \\ & & & A_p \end{bmatrix}$$

$$A = K_t \otimes M_h + M_t \otimes K_h, \qquad A_p = M_t \otimes K_h$$



Conclusions

- Current Work
  - Symbol–based smoothing
  - Space–time Adaptivity
  - Scaling experiments on bigger machines

Thank you!

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