Efficient implementation of polytopal Discontinuous Galerkin methods with application to multilevel solvers

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deal.II workshop, 13 Aug 2024
Fort Collins (CO)

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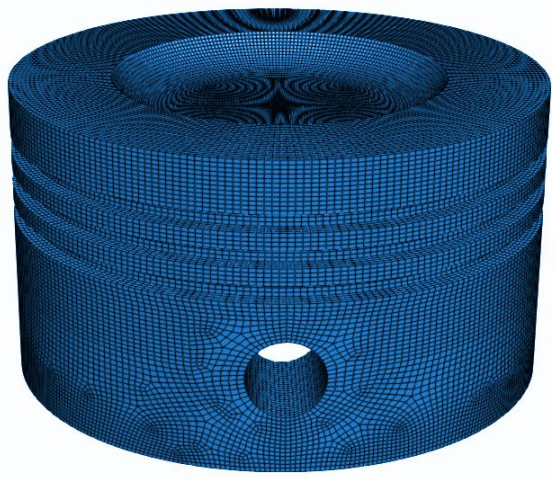
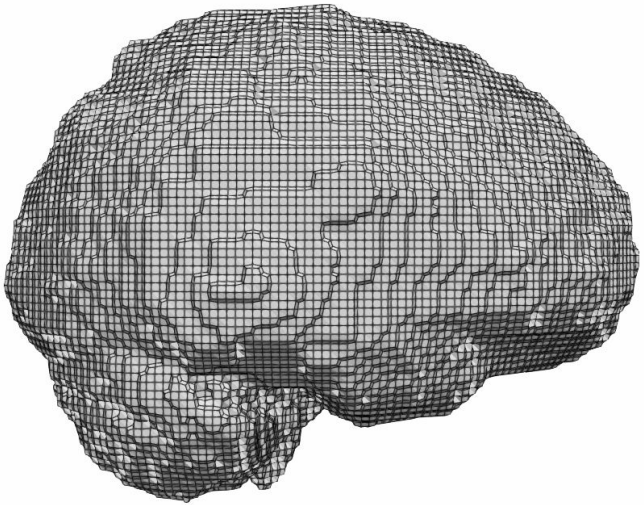
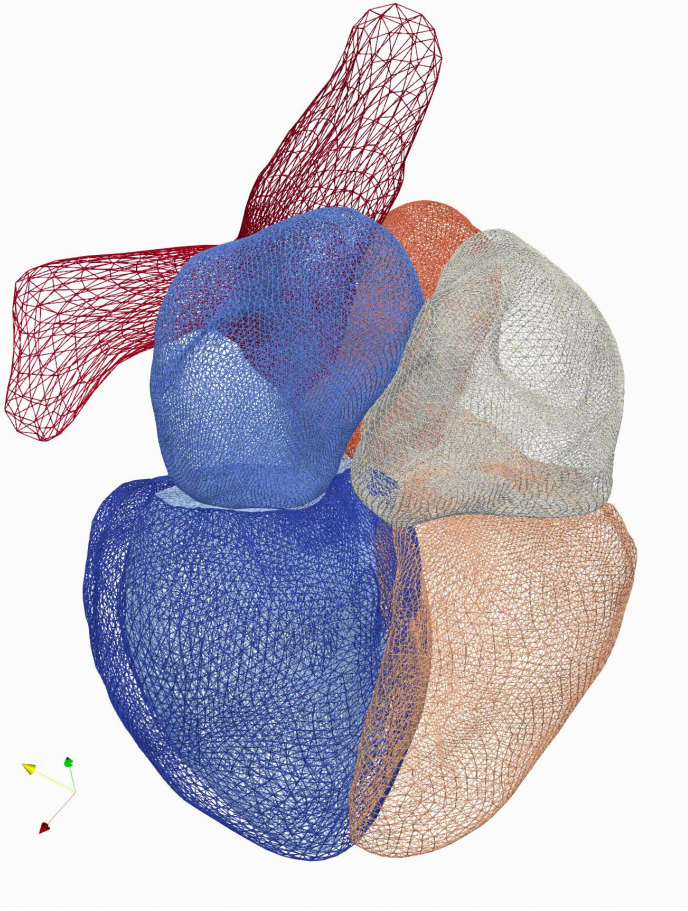
Outline

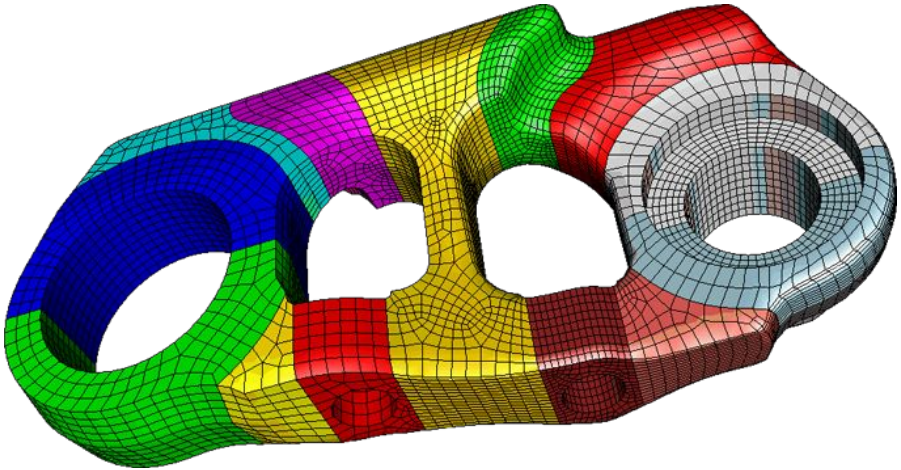
1. Motivation
2. R-tree data structure for FEM
3. Mesh agglomeration: METIS vs. R-tree
4. Polytopal DG + Agglomerated GMG
5. Implementation + parallelization strategies
6. Application to cardiac electrophysiology

Motivation









Motivation

- Traditional Finite Element Methods (FEMs) may struggle to accurately represent complex geometries coming from real-world applications.
- Grid generation is often a bottleneck due to the limitations of using only tetrahedral, hexahedral, or prismatic elements.
- Polytopal methods (polygonal FEM, mimetic FD, VEM, PolyDG, HDG, HHO) have shown to be particularly effective in representing complex geometries.
- Polytopal methods are attractive in this respect since *coarse* grids can be simply generated by merging polygonal and polyhedral elements.

➔ Providing automated and good-quality **agglomeration strategies** for polygonal and polyhedral elements remains an open and challenging task.

➔ It is indeed crucial to **preserve the original mesh quality**, as any deterioration could potentially affect the overall performance of the method in terms of **stability and accuracy**.


WHO ARE WE?
DEAL.II USERS
WHAT DO WE WANT?
SIMULATIONS
OF COMPLEX MODELS
WHEN DO WE WANT IT?
YESTERDAY!
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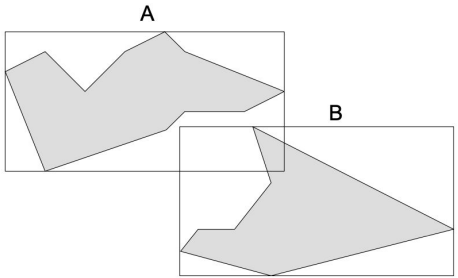
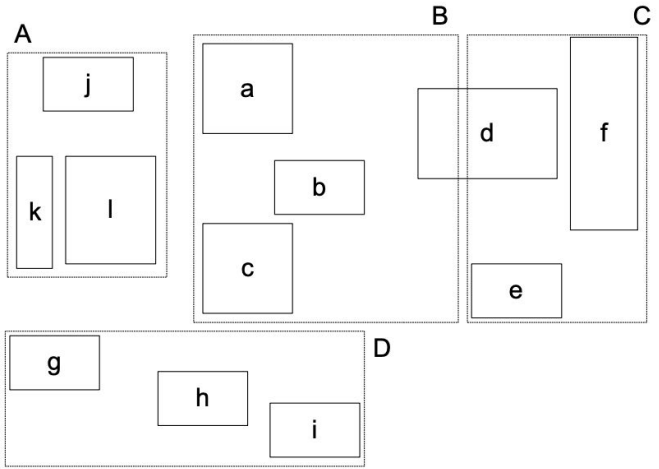
R-tree data structure for FEM

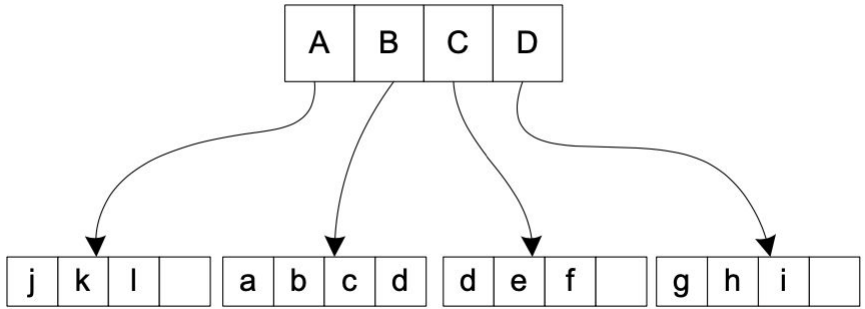
R-tree data structure

- Used for the dynamical organisation of generic geometric objects
- Objects represented by their bounding box



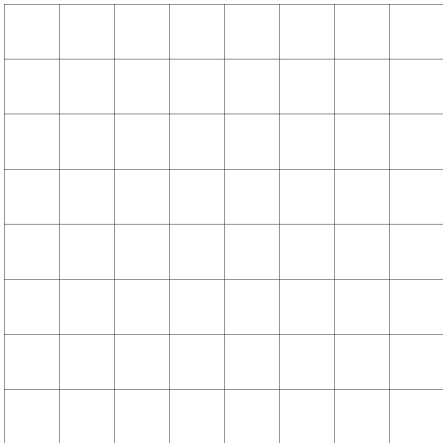


- Leaves of the tree: real objects
- Internal node stores:
  - *Pointer* to child node
  - *Box* of all entries within child node

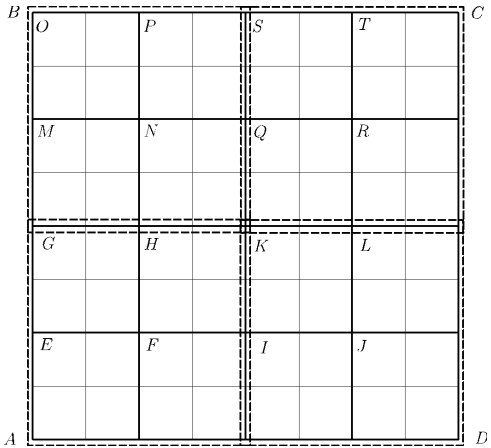


R-tree and finite elements

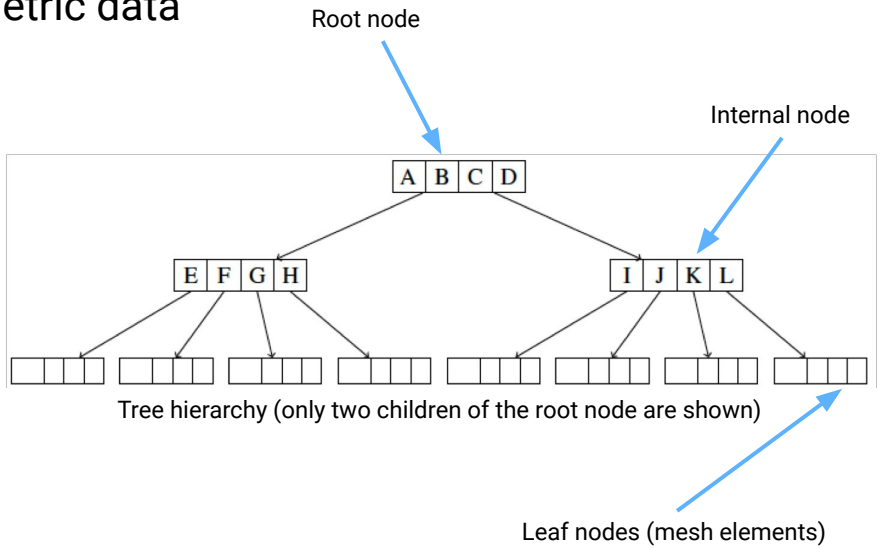
- Basic idea: use mesh elements as the geometric data
- Represents object by their bounding box



Original 8x8 mesh $(0, 1)^2$



Bounding boxes and mesh elements



- **A** has child node with entries: **E**, **F**, **G**, **H**
- Each box bounds 4 mesh elements

Mesh agglomeration: METIS vs. R-tree

Agglomeration strategy

Overall procedure

- *Build* R-tree out of bounding boxes $\{\text{BBOX}(T_i)\}_{i=1,\dots,N}$
- *Select* target level $l \in \{1, \dots, L\}$
- For every node on level, *descend* recursively its children until leaf nodes are reached
- *Agglomerate* together leaf nodes sharing the same ancestor

- Proper parent-child relationships
- Generate sequence $\{\mathcal{T}_k\}_k$ of nested, *agglomerated*, meshes for **multilevel methods**
- Intergrid transfers are cheap: canonical injection between nested spaces (cfr. non-nested multigrid)

- We compare to METIS, popular way to generate polytopic meshes

Algorithm 1 Creation of agglomerates.

Input: R-tree R of order (M, m)
Input: $l \in \{1, \dots, L\}$ target level.
Output: v vector s.t. $v[n]$ stores leafs associated to node n

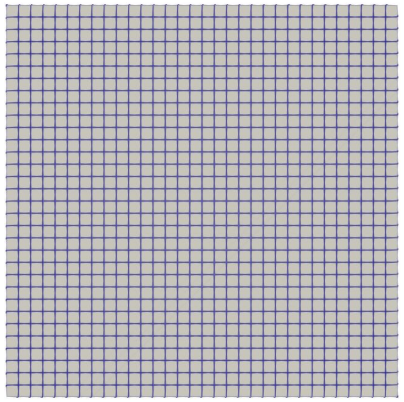
```
1: function ComputeAgglomerates(R, l)
2:     for node n in N_l do
3:         v[n] ← ExtractLeafs(l, n)
4:     end for
5: end function
```

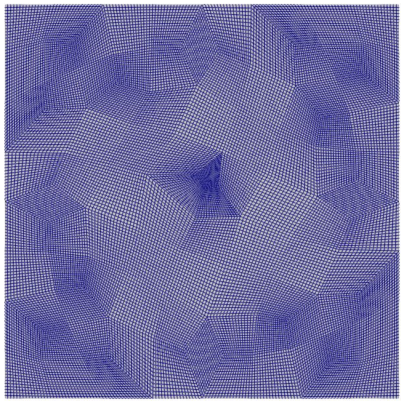
Algorithm 2 Recursive extraction of leafs from a node n on level l.

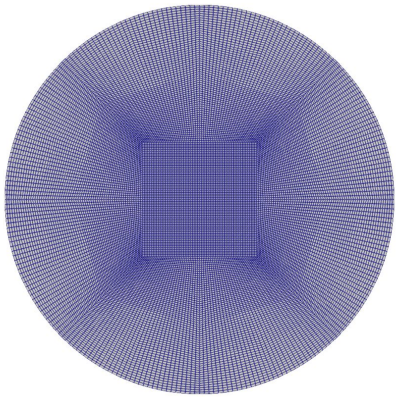
Input: $l \in \{1, \dots, L\}$ target level
Input: $n \in N_l$
Output: vector $v[n]$ containing leafs which share the ancestor node n.

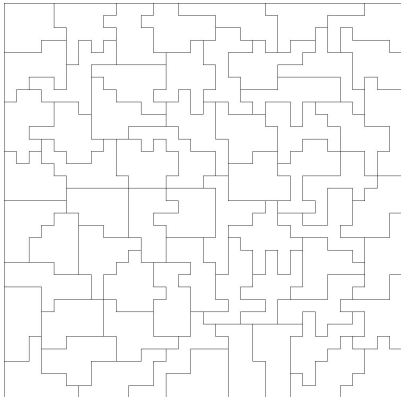
```
1: function ExtractLeafs(l, n)
2:     if l = 1 then
3:         v[n] ← {T_n^1, ..., T_n^M}
4:     else
5:         ExtractLeafs(l − 1, n)
6:     end if
7: end function
```

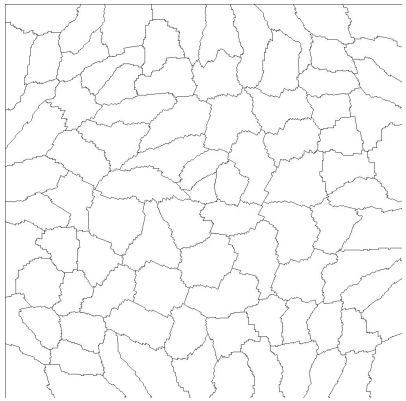
2D examples (METIS – graph *k*-way)

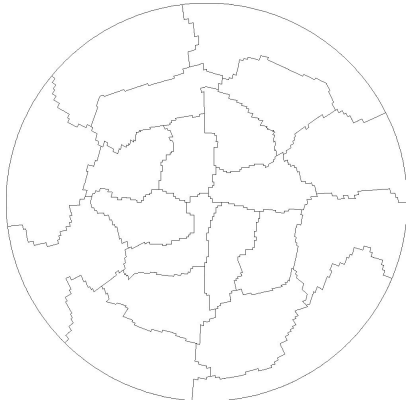




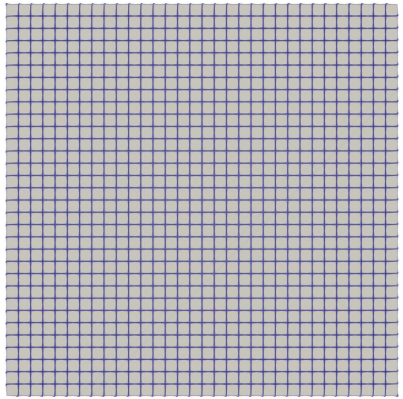


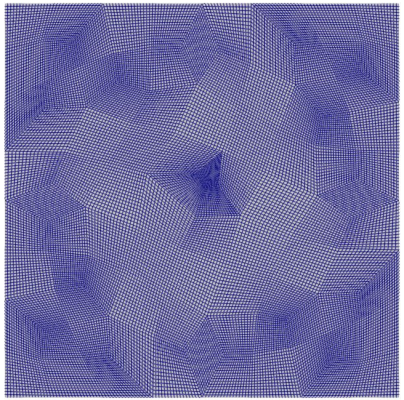


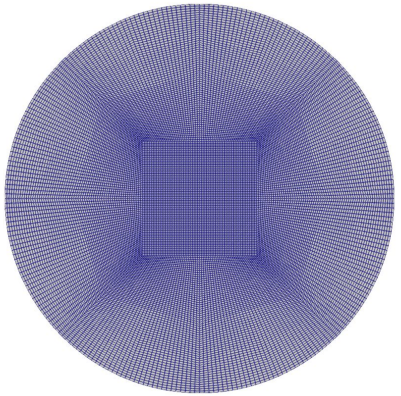


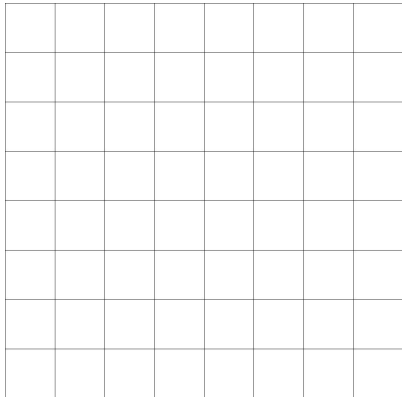


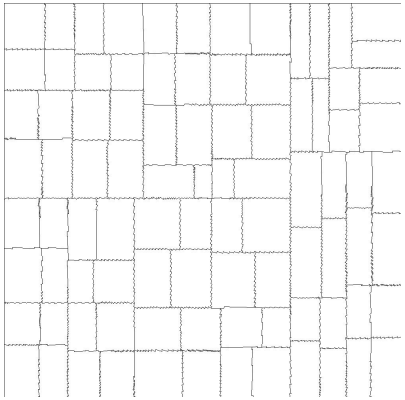
2D examples (R-tree)

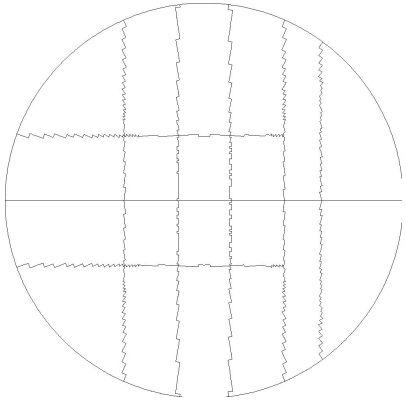




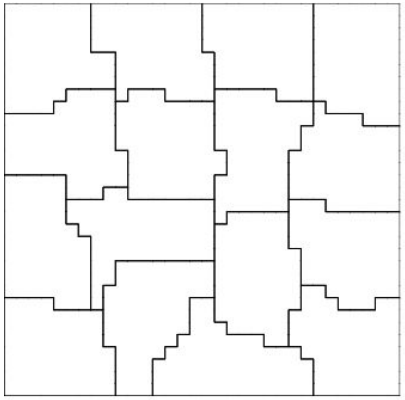




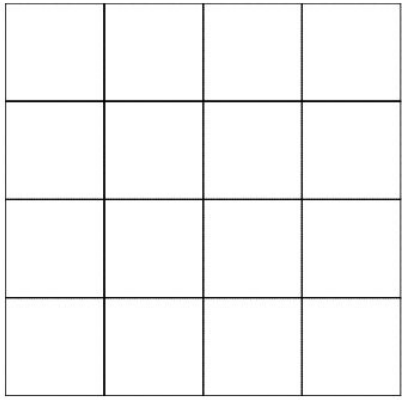




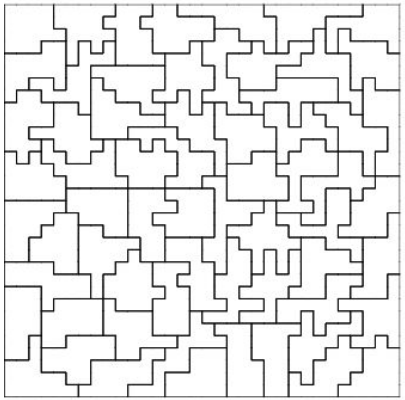
2D example: structured square



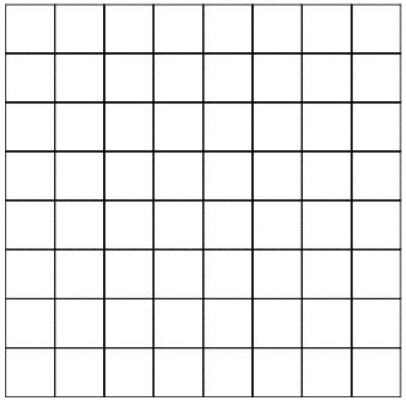
(a) METIS, n_partitions = 16.



(b) R-tree, extraction_level = 2.



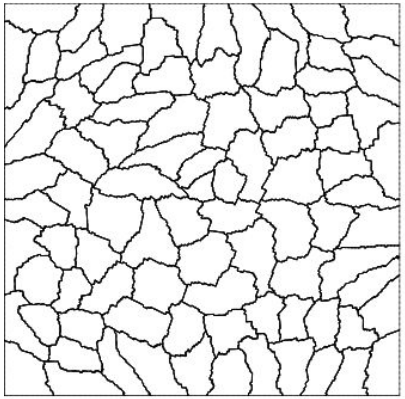
(c) METIS, n_partitions = 64.



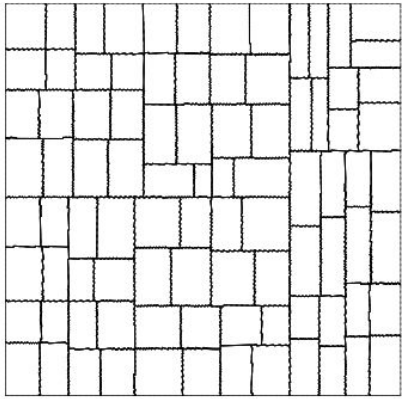
(d) R-tree, extraction_level = 3.

METIS: Geometrical features not preserved!

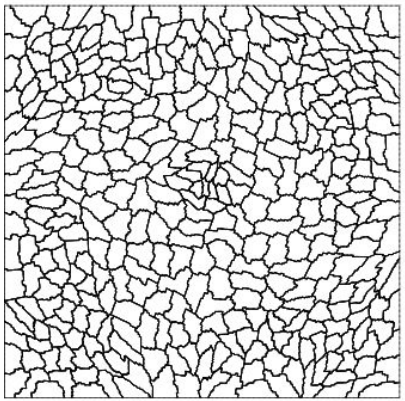
2D example: unstructured square



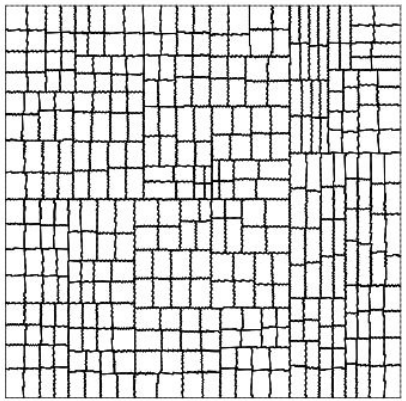
(a) METIS, `n_partitions` $= 91$.



(b) R-tree, `extraction_level` $= 4$.

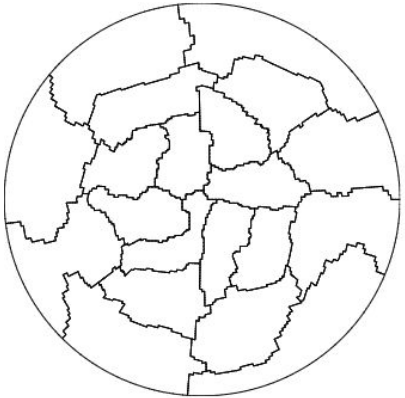


(c) METIS, `n_partitions` $= 364$.

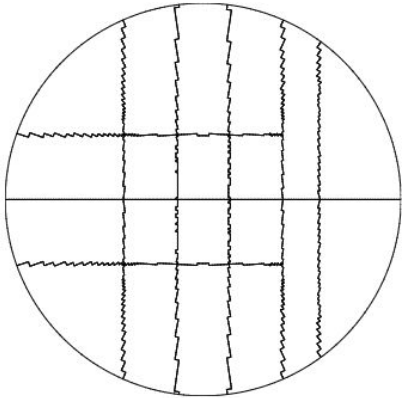


(d) R-tree, `extraction_level` $= 5$.

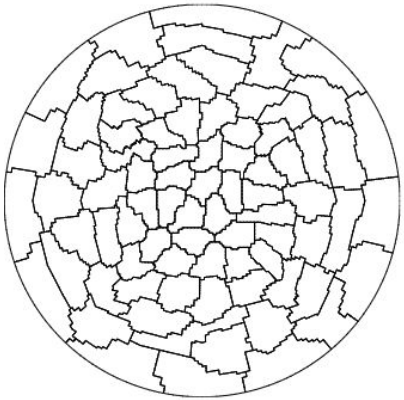
2D example: structured ball



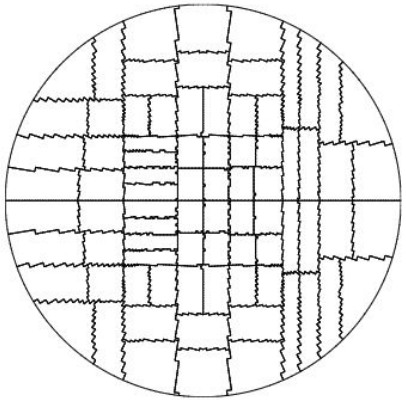
(a) METIS, `n_partitions` = 20.



(b) R-tree, `extraction_level` = 3.

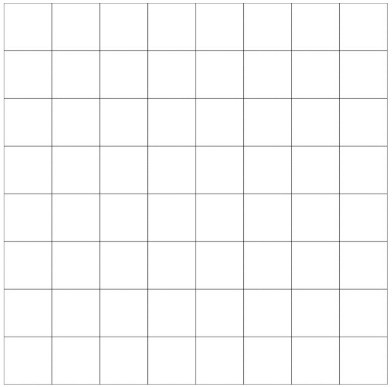


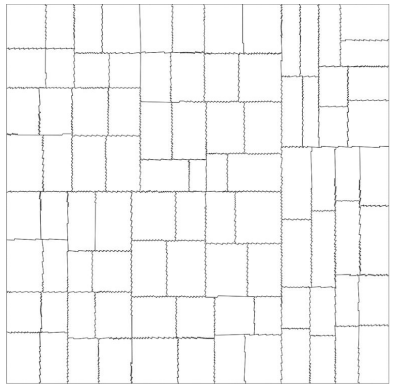
(c) METIS, `n_partitions` = 80.

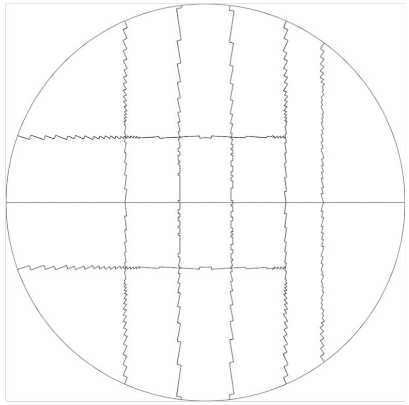


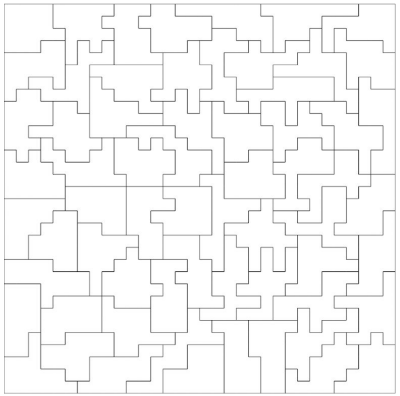
(d) R-tree, `extraction_level` = 4.

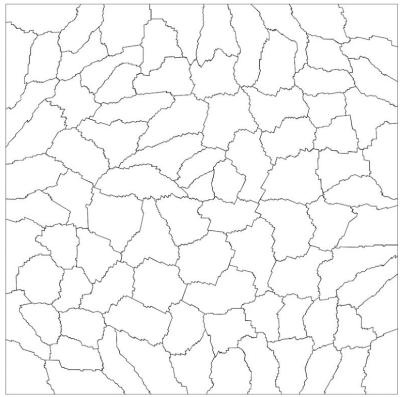
Visual comparison

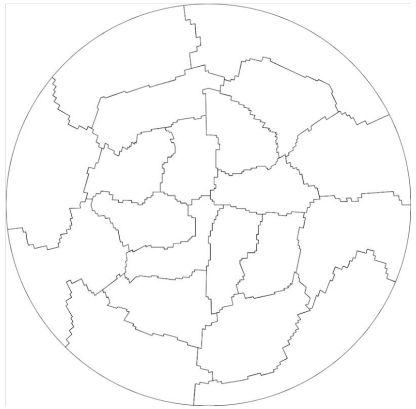












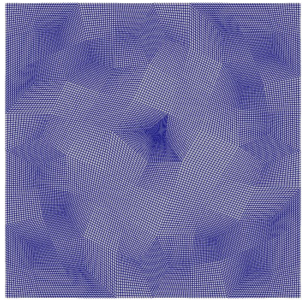
R-tree strategy:

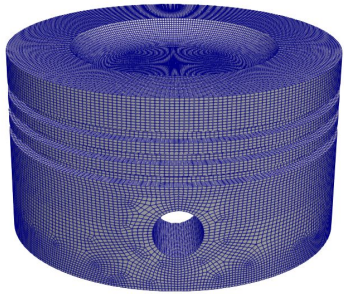
- Produces agglomerates tightly close to each bounding box
- Preserves geometrical features
- Better quality indicators for polytopal elements (uniformity ratio, circle ratio, box ratio)

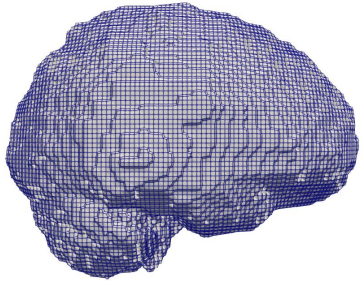
How *fast* is it?

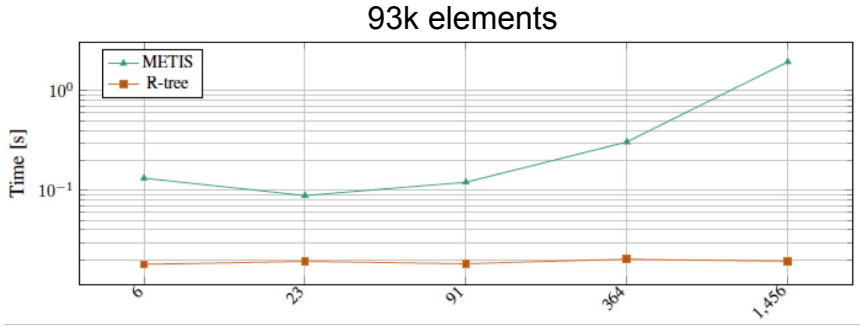
- We measure wall-clock time against graph *k*-way algorithm implemented by METIS

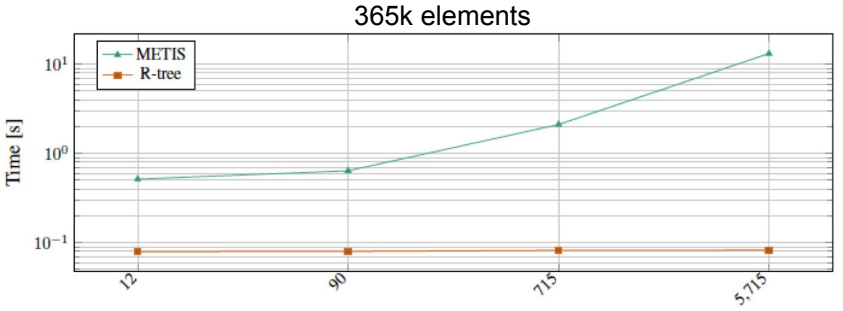
- We time (cumulatively):
  - Building the R-tree
  - Visiting tree and the hierarchy
  - Flagging original mesh cells

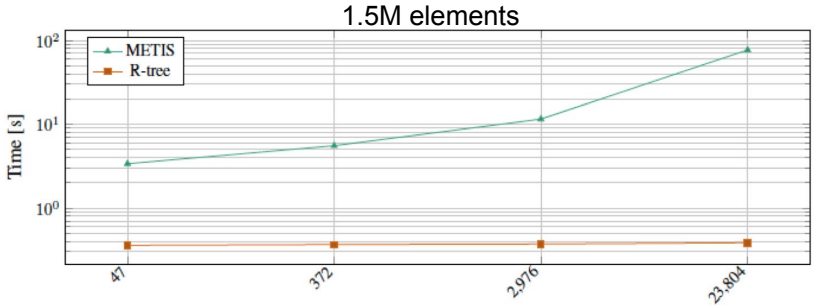












R-tree: targets and properties

Targets

- Minimisation of area covered by each box
- Minimisation of overlap between boxes
- Minimisation of boxes' perimeters

Several possible variants.
Choice: ***R*-tree***

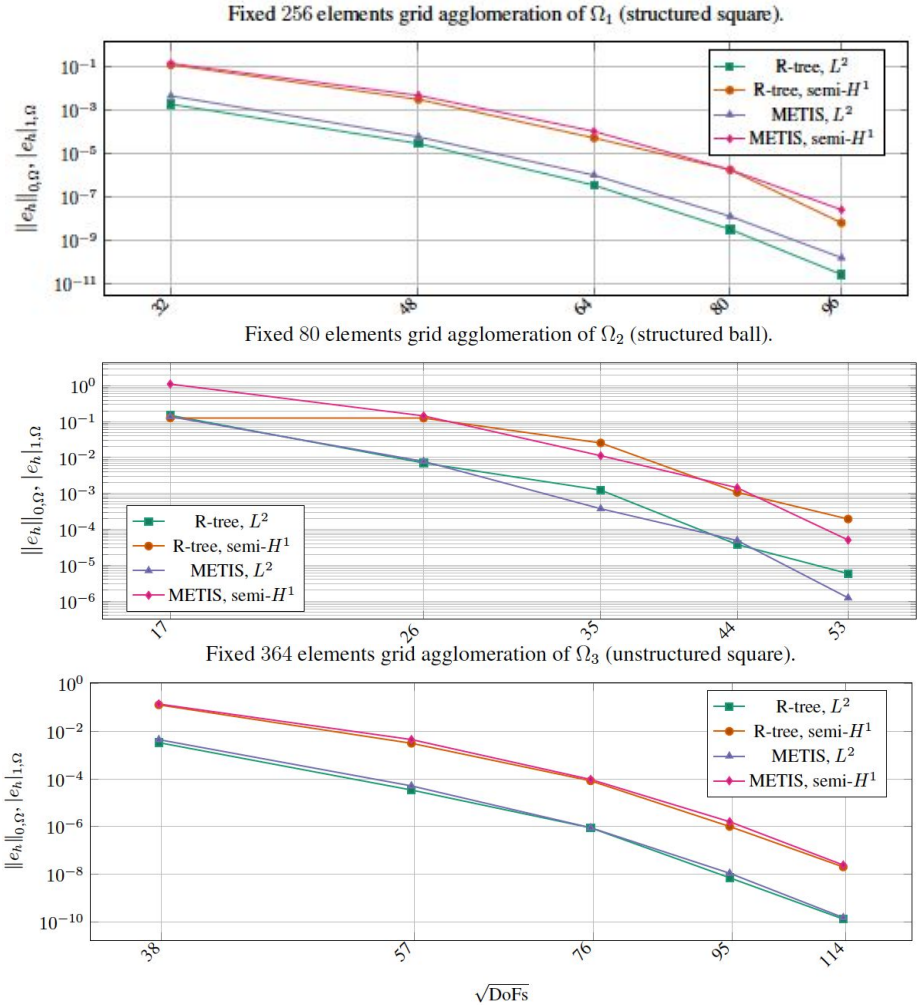
Properties

- R-tree shows constant wall-clock times
- *Independent* of the extraction level *l*
- R-tree manipulation:
  - Relies on `Boost.Geometry` library
  - Hierarchy traversal *not* natively supported
  - Requires implementation of node *visitor*

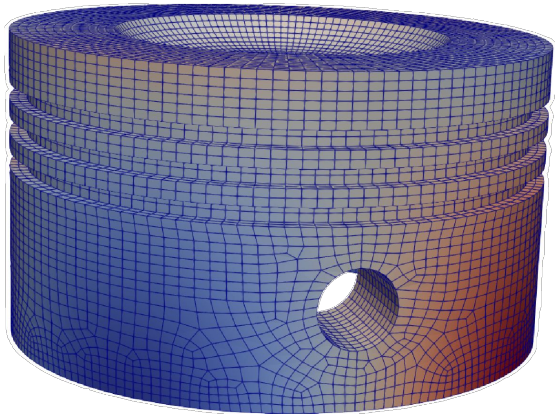
Polytopal DG + Agglomerated GMG

Polytopal DG

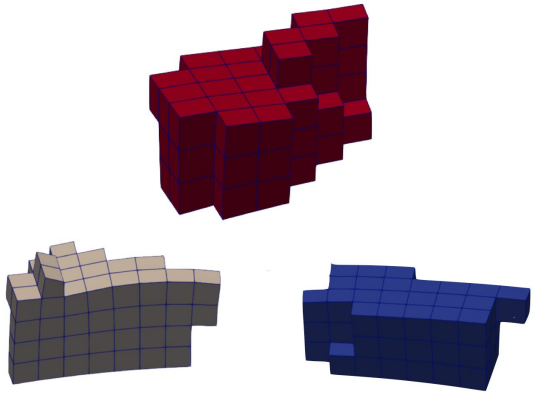
- Discontinuous nodal space defined on bounding boxes
- *p*-convergence for a simple diffusion-reaction equation
- Quadrature formulas coming from sub tessellation, readily available from underlying mesh



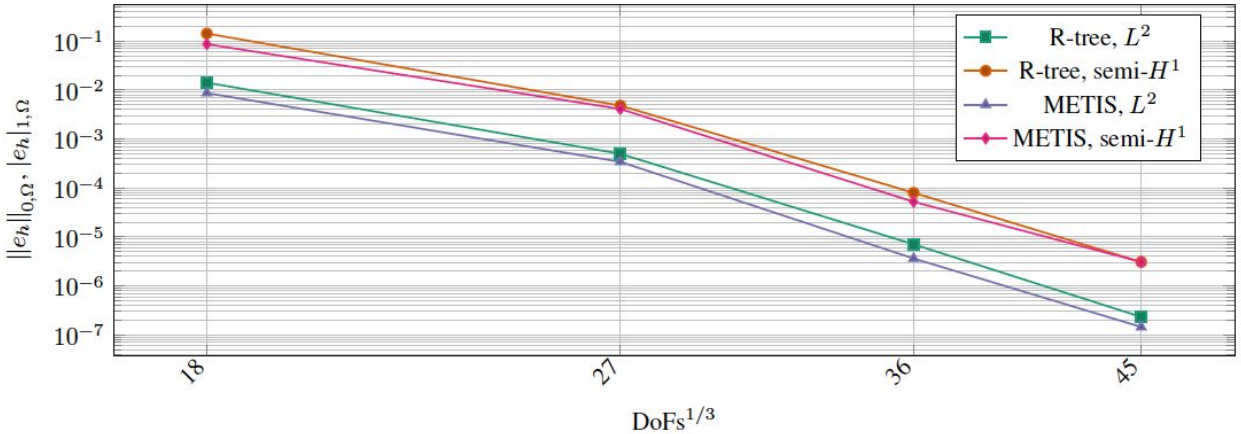
Polytopal DG: 3D piston model



	Number of DoFs	
p	Number of DoFs (original mesh)	Number of DoFs (agglomerated mesh)
1	365,712	25,425
2	1,234,278	48,366
3	2,925,696	108,492
4	5,714,250	175,020



Fixed 731 elements grid agglomeration of 3D piston model.



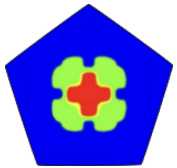
Implementation + parallelization strategies

Implementation

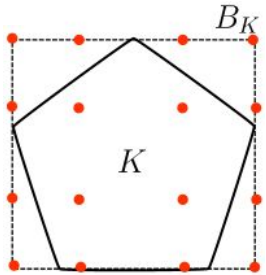
- Open-source C++ library `polyDEAL`: https://github.com/fdrmrc/Polydeal
- Builds on top of the `deal.II` library
- PETSc & `Trilinos` as linear algebra backends
- Distributed memory implementation handled through MPI
- Minimal changes required:
  `DoFHandler<dim>` → `AgglomerationHandler<dim>`
- Memory-distributed agglomerated multigrid
- Iterators on mesh-like containers:

```
for (const auto &polytope : agglomeration_handler.active_polytope_iterators())
  {
    if (polytope->is_locally_owned())
      {
        // do stuff with polytope
      }
  }
```

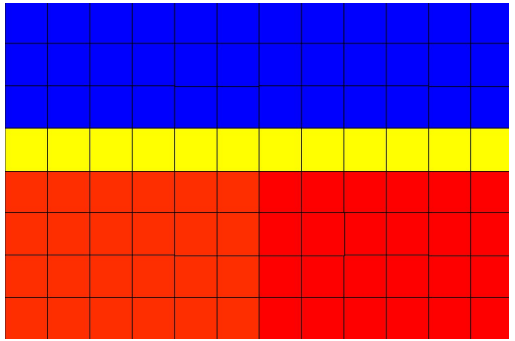
```
for (const auto &cell : dof_handler.active_cell_iterators())
  {
    if (cell->is_locally_owned())
      {
        // do stuff
      }
  }
```



Parallelization strategies



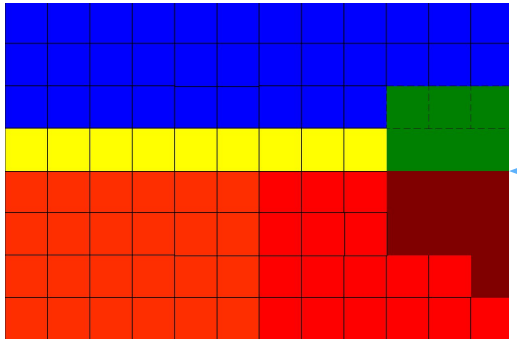
- Standard nodal DG space over the bounding box of each polytope
- Agglomeration is performed within each locally owned partition



Rank 0

Ghost

Rank 1



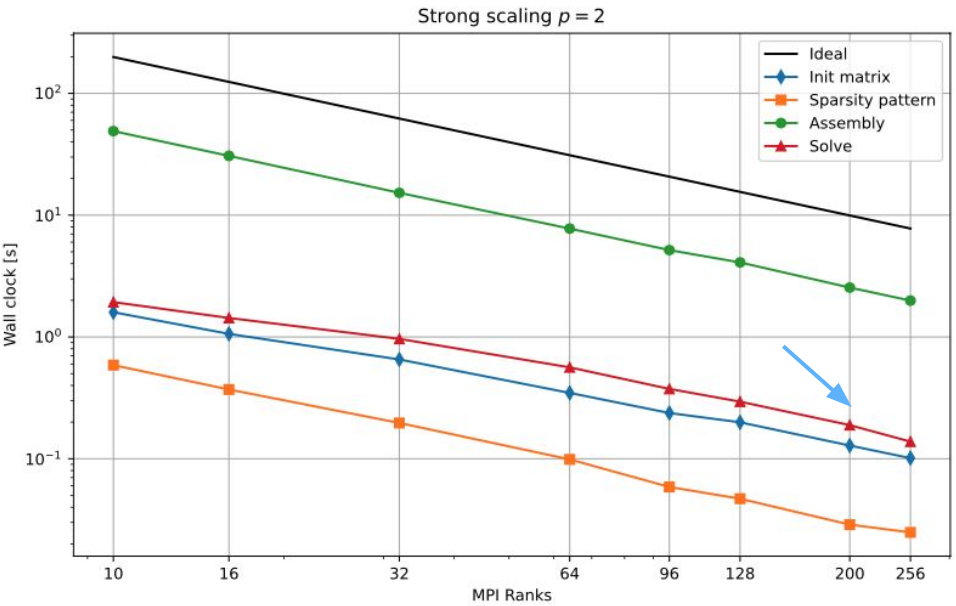
- Green polytope is ghosted
- Sub-elements are in general remote

- Flux DG terms require knowledge of metadata that are *not* just ghosted, but *fully* remote
- MPI non-blocking communication during setup phase on processors' boundaries

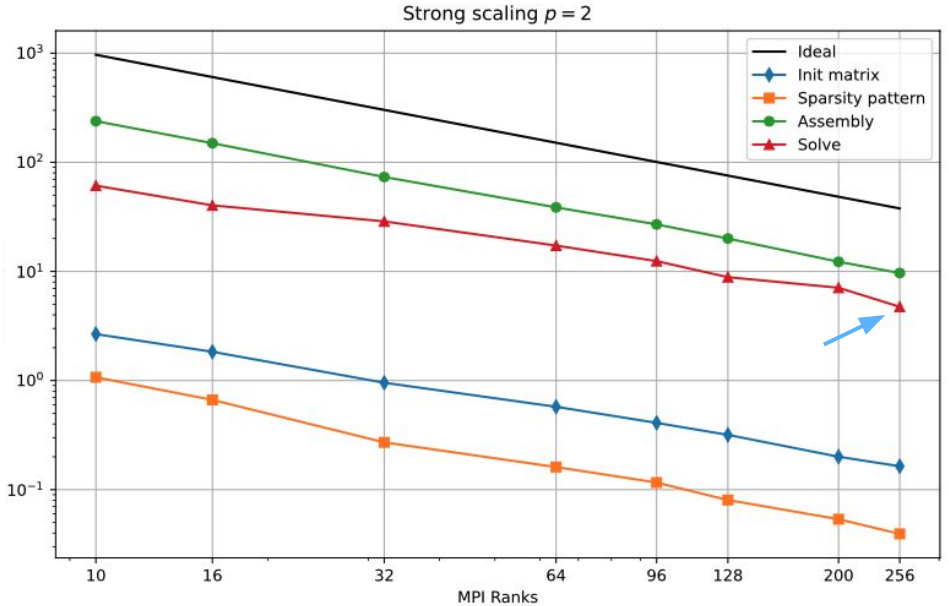
Benchmarks

- $-\Delta u = f$ on unit cube, Q^2 elements
- Solver: CG + AMG (`TrilinosML`)
- Complexity shifted to assembly phase

From **262k** original hexas → **7k** agglomerates

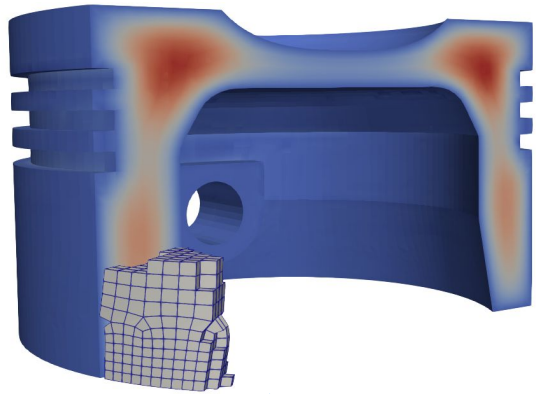


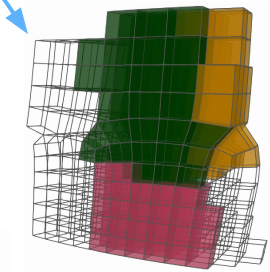
From **2.7m** original hexas → **70k** agglomerates

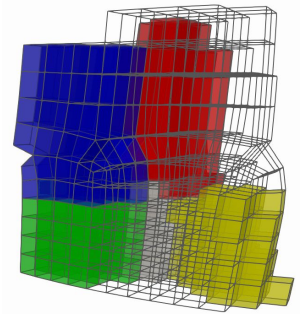


Agglomerated MultiGrid

- Basic idea: *use agglomeration to build coarser operators*
- Keep original mesh as finest level
- Use agglomerates just to create intergrid transfers $\{P_{l+1}^l\}_l$
- Start from $A_0 = \frac{M}{\Delta t} + A$
- Build coarser operators algebraically using $A_{l+1} = \left(P_{l+1}^l\right)^T A_l P_{l+1}^l$
- No need to assemble on each level
- Trivial to add in existing multigrid framework







Unstructured square

levels \ p	1	2	3	4	5
4	9	10	11	11	14
5	10	10	11	12	14
6	10	10	11	12	14

Piston

levels \ p	1	2	3	4
4	9	11	14	15
5	10	11	14	16
6	10	11	14	16

CG + MG iteration counts for SIPDG

Application to cardiac electrophysiology

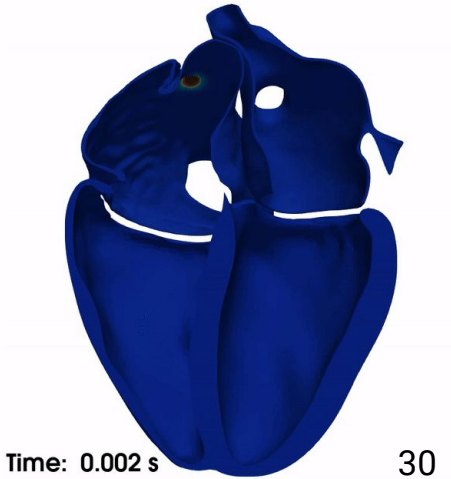
Cardiac electrophysiology in a nutshell

$$
\begin{cases}
\chi\left(C_{\mathrm{m}}\dfrac{\partial u}{\partial t}+\mathcal{I}_{\mathrm{ion}}(u,\boldsymbol{w},\boldsymbol{z})\right)-\nabla\cdot(\boldsymbol{D}_{\mathrm{M}}\nabla u)=\chi\mathcal{I}_{\mathrm{app}}(\mathbf{x},t), & \text{in } \Omega\times(0,T],\\
(\boldsymbol{D}_{\mathrm{M}}\nabla u)\cdot\mathbf{n}=0, & \text{on } \partial\Omega\times(0,T],\\
\dfrac{d\boldsymbol{w}}{dt}=\boldsymbol{H}(u,\boldsymbol{w},\boldsymbol{z}), & \text{in } \Omega\times(0,T],\\
\dfrac{d\boldsymbol{z}}{dt}=\boldsymbol{G}(u,\boldsymbol{w},\boldsymbol{z}), & \text{in } \Omega\times(0,T],\\
u(\mathbf{x},0)=u_0(\mathbf{x}),\ \boldsymbol{w}(\mathbf{x},0)=\boldsymbol{w}_0(\mathbf{x}),\ \boldsymbol{z}(\mathbf{x},0)=\boldsymbol{z}_0(\mathbf{x}), & \text{in } \Omega.
\end{cases}
$$

Motivation:

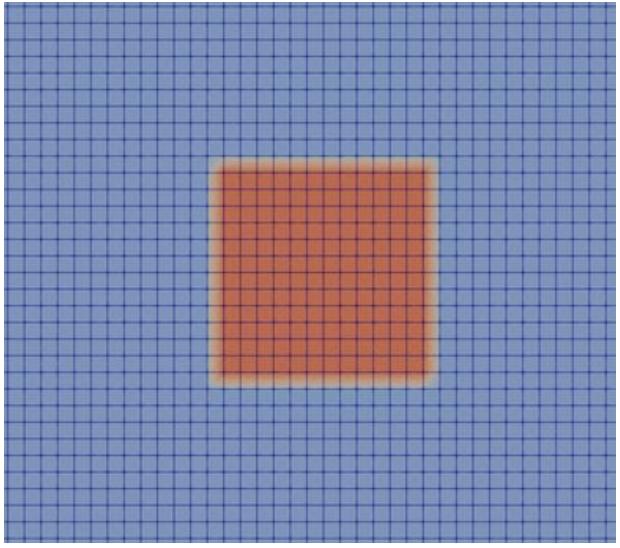
- solution characterized by a sharp and fast propagating wavefront
- extreme numerical accuracy (in space/time) required
- high−dimensional problems

→ **need for a high performance solver**



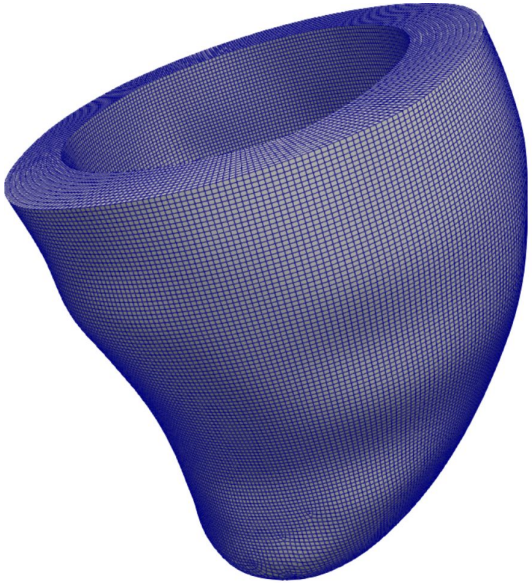
Application to cardiac electrophysiology

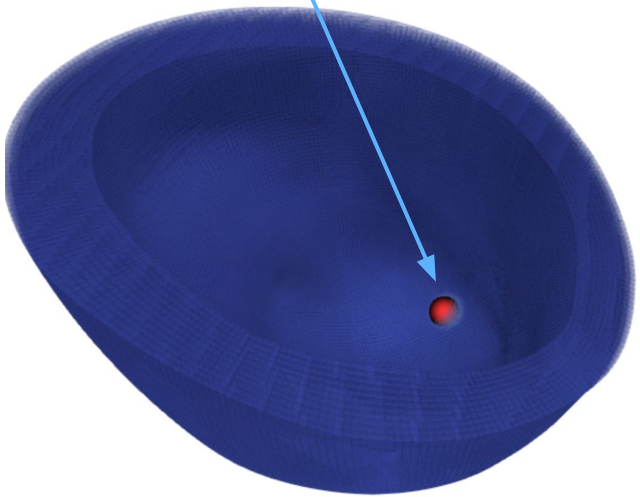
- Monodomain problem with high order DG
- Exploit polytopic/agglomerated multigrid to precondition the resulting DG system
- 4 levels with ~90, 360, 720 elements.
- Polynomial order 3 → ~8 iterations/time step (≪ AMG).

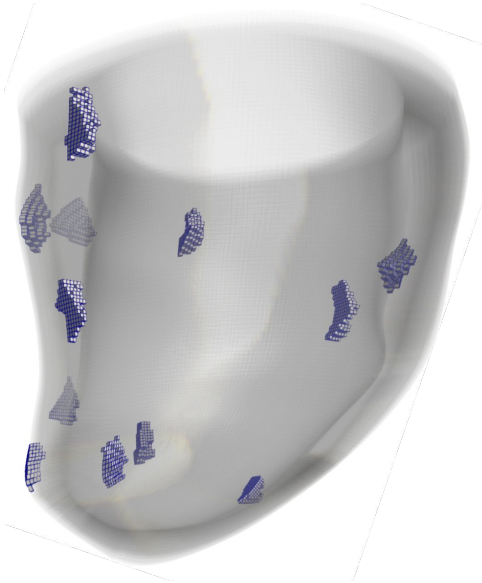


Application to cardiac electrophysiology

- Realistic mesh of left ventricle (370k hexas)
- View of some of the agglomerates
- Apply impulse at specific points







Application to cardiac electrophysiology

- Semi-implicit discretization yields

$$\left(\frac{M}{\Delta t} + A\right)\boldsymbol{U}_{n+1} = MI^h_{app,n+1} - MI^h_{ion}(\boldsymbol{U}_n, \boldsymbol{W}_{n+1}) + \frac{M}{\Delta t}\boldsymbol{U}_n$$

- Preconditioned conjugate-gradient with agglomerated multigrid
- Only need the operator evaluation on the fine level

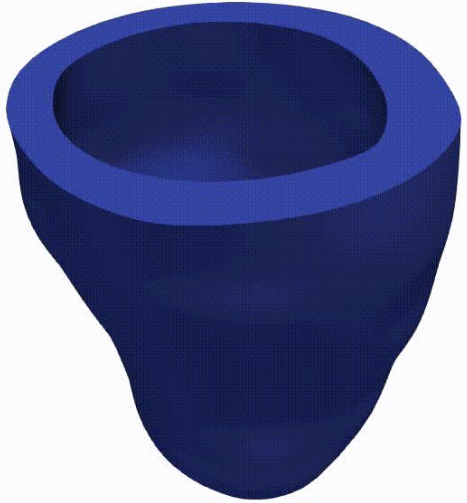
- Ratio close to 8
- Well balanced levels

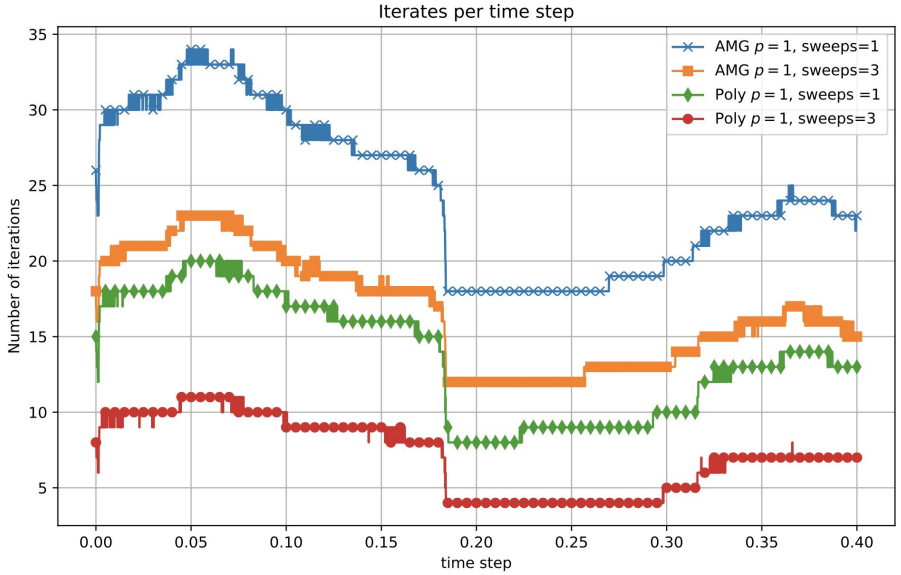
Hierarchy for ventricle mesh (**128** processors)		
Level l	Card($\mathcal{T}_l$)	Card($\mathcal{T}_{l-1}$)/Card($\mathcal{T}_l$)
$l = 0$	374 022	–
$l = 1$	46 809	~ 7.9
$l = 2$	5 908	~ 7.9
$l = 3$	768	~ 7.7

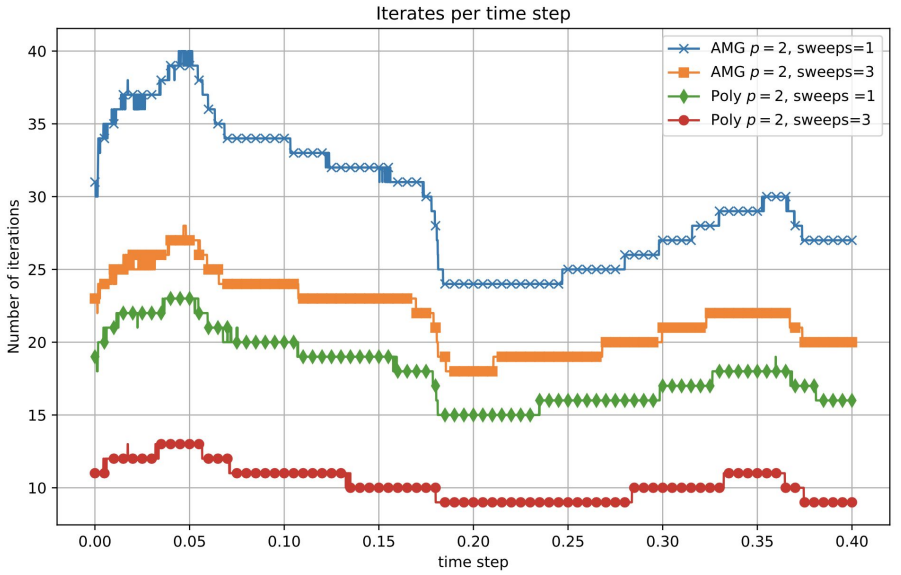
Hierarchy for ventricle mesh (**256** processors)		
Level l	Card($\mathcal{T}_l$)	Card($\mathcal{T}_{l-1}$)/Card($\mathcal{T}_l$)
$l = 0$	374 022	–
$l = 1$	46 871	~ 7.9
$l = 2$	5 987	~ 7.8
$l = 3$	768	~ 7.8

Iteration counts

- Solve until $T = 0.4s$, with $\Delta t = 10^{-4}s$
- Lower iteration counts compared to CG+AMG
- Robust with respect to number of levels and MPI ranks







Outlook and future work

- ✓ Distributed implementation of polyDG and agglomerated MG
- ✓ Successfully applied to large geometries
- ✓ Application to cardiac electrophysiology
- ⏲ Matrix-free operator evaluation

References

[1] A. Guttmann - R-Trees: a Dynamic Index Structure for Spatial Searching (1984).

[2] P. F. Antonietti, M. Sarti, M. Verani - Multigrid algorithms for hp-version interior penalty discontinuous Galerkin methods on polygonal and polyhedral meshes (2015).

[3] A. Cangiani, Z. Dong, E. H. Georgoulis - hp-Version discontinuous Galerkin methods on essentially arbitrarily-shaped elements (2022).

[4] PCA, M. Salvador, P. Gervasio, L. Dede', A. Quarteroni - A matrix-free high-order solver for the numerical solution of cardiac electrophysiology (2023).

[5] M. Feder, A. Cangiani, L. Heltai - R3MG: R-tree based agglomeration of polytopal grids with applications to multilevel methods (2024).

Research funded by:

- NextGenerationEU (project ID ECS_00000043)

Thanks!

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