Compatible and reliable numerical modelling with PDEs

Andrea Cangiani

mathLab, Mathematics Area, SISSA

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SISSA mathLab

The SISSA mathLab is a laboratory for mathematical modelling and scientific computing.

- part of Mathematics Area
- funded in 2010
- 5 professors, many research associates and PhD students
- What we do:
  - Interaction between mathematics and its applications
  - From theoretical numerical analysis to industrial projects
  - High Performance Computing
  - Open Source Software Development

Se also talks by Giovanni Noselllli and Davide Torlo (Wednesday)

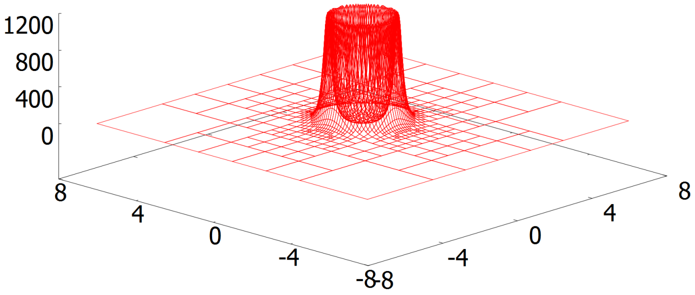
Research area

- Continuum modelling with Partial Differential Equations (PDEs), eg. in biomedicine, geophysics, engineering
  - Interaction of different phenomena (*eg.* transport and diffusion)
  - Non-linear effects (*eg.* flux through semipermeable membranes)
- Development & analysis of new numerical PDE methods, HPC
  - Finite Element-type methods on general meshes
  - Automatic adaptivity driven by reliable a posteriori error estimation

Reliable. I exist, hence I compute! [C, Kyza, Georgoulis, Metcalfe, SISC, 2016]

A nonlinear problem with finite-time blow-up: $\partial_t u - \kappa \Delta u + \mathbf{b} \cdot \nabla u = u^2$

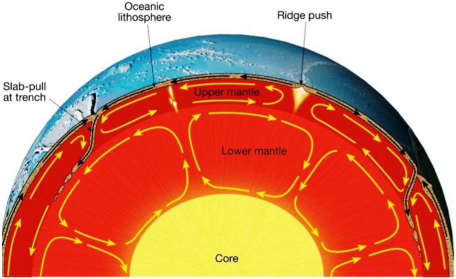
- Analytical results: blowup time?
- Standard numerical methods: prohibitive resolol ution required
- Mesh-adaptive methods driven by conditional[1] a posteriori error control $\rightarrow$ used to drive guaranteed adaptive computations



[1] hold under some computationally verifiable conditions

Compatible. A space-time journey to the centre of earth

Reverse-engineering the history of earth's continental plates



- Long timescale calculation - 100My+
- Capture fine features on whole mantle
- Multiple runs - inverse problem

Simplified Boussinesq model of convection

$$
\begin{aligned}
-\nabla \cdot (\mu(T)(\nabla \mathrm{u} + \nabla \mathrm{u}^{\mathrm{T}})) + \nabla p &= -\rho(T)\mathrm{g} \\
\nabla \cdot \mathrm{u} &= 0 \\
T_t - \varepsilon \Delta T + \mathrm{u} \cdot \nabla T &= f
\end{aligned}
$$

Adaptive large-scale earth mantle convection simulations

Parallel implementation of Boussinesq model embedded into community code ASPECT **[Bangerth et al. 2018]**:

- Taylor-Hood + discontinuous Galerkin FEM
- Adaptivity via residual-based a posteriori error estimator
- load-balancing operation

van Kenen benchmark **[S. Cox, PhD thesis, Leicester, 2016]**.

Variational problems and the Ritz-Galerkin method

Abstract variational (linear) problem: Find $u \in V$:

$$A(u, v) = F(v) \qquad \forall v \in V$$

Stokes problem with homogeneous Dirichlet b.c.

Find $(\mathrm{u}, p) \in \mathrm{H}_0^1(\Omega) \times L^2(\Omega) \setminus \mathbb{R}$:

$$\begin{aligned} -\Delta \mathrm{u} + \nabla p &= \mathrm{f} \qquad \text{in } \Omega, \\ \nabla \cdot \mathrm{u} &= 0 \qquad \text{in } \Omega. \end{aligned}$$

Variational problem: find $(\mathrm{u}, p) \in \mathrm{H}_0^1(\Omega) \times L^2(\Omega) \setminus \mathbb{R}$:

$$\begin{aligned} a(\mathrm{u}, \mathrm{v}) + b(\mathrm{v}, p) &= (\mathrm{f}, \mathrm{v}) \qquad \forall \mathrm{v} \in \mathrm{H}_0^1(\Omega), \\ b(\mathrm{u}, q) &= 0 \qquad \forall q \in L^2(\Omega) \setminus \mathbb{R}. \end{aligned}$$

with $a(\mathrm{u}, \mathrm{v}) = \int_\Omega \nabla \mathrm{u} : \nabla \mathrm{v}$, $b(\mathrm{v}, p) = \int_\Omega p \nabla \cdot \mathrm{v}$, and $(\mathrm{f}, \mathrm{v}) = \int_\Omega \mathrm{f} \cdot \mathrm{v}$.

Variational problems and the Ritz-Galerkin method

Abstract variational (linear) problem: Find $u \in V$:

$$A(u, v) = F(v) \qquad \forall v \in V$$

Let $V_n \subset V$ some n-dim *conforming* subspace.

Ritz-Galerkin method: Find $u_n \in V_n$:

$$A(u_n, v) = F(v) \qquad \forall v \in V_n$$

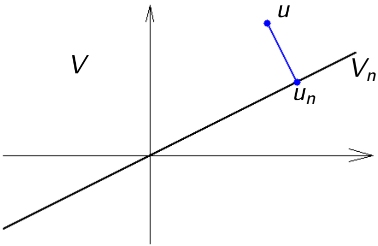
Consistency (Galerkin Orthogonality):

$$A(u - u_n, v_n) = 0 \quad \forall v_n \in V_n.$$

If V is Hilbert with Inner Product

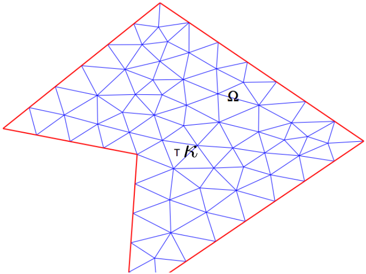
$$[u, v] := A(u, v)$$

then u_n is the projection of u onto V_n!

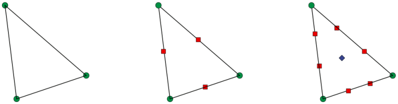


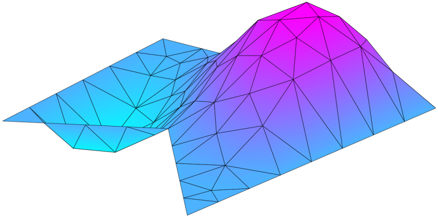
Finite Element Methods

- Split the problem domain $\Omega \subset \mathbb{R}^d$ into elements $\kappa \in \mathcal{T}$ where $\mathcal{T}$ denotes the mesh.
  Standard elements are triangular or quadrilateral.



- Pick an appropriate finite element space V_n of piecewise polynomials.





Why polynomials?

- Easy to compute with
- Known approximation properties

Why triangles/quadrilaterals?

- Easy to glue local spaces continuously across edges

Some FEM for the Stokes system

Taylor-Hood (1973): $\mathcal{P}^d_{p+1}(\kappa) \times \mathcal{P}_p(\kappa)$, triangular elements, global spaces

$$\mathsf{U}_n \times \mathrm{P}_n \subset \mathsf{H}^1_0(\Omega) \times L^2(\Omega)$$

Consistent and conforming but the solution u_n is not necessarily div-free.

BDM-DG [Cockburn-Kanschat-Schotzau (2007), Schotzau et al. (2014)]: $\mathcal{P}^d_{p}(\kappa) \times \mathcal{P}_{p-1}(\kappa)$,

$$\mathsf{U}_n \times \mathrm{P}_n \not\subseteq H^1_0(\Omega) \times L^2(\Omega)$$

$$a_n(\mathsf{u}_n, \mathsf{v}_n) = \sum_{\kappa \in \mathcal{T}} \int_\kappa \nabla \mathsf{u}_n : \nabla \mathsf{v}_n - \int_\Gamma (\{\nabla \mathsf{u}_n\} \cdot [\mathsf{v}_n] + \{\nabla \mathsf{v}_n\} \cdot [\mathsf{u}_n] - \sigma [\mathsf{u}_n][\mathsf{v}_n])$$

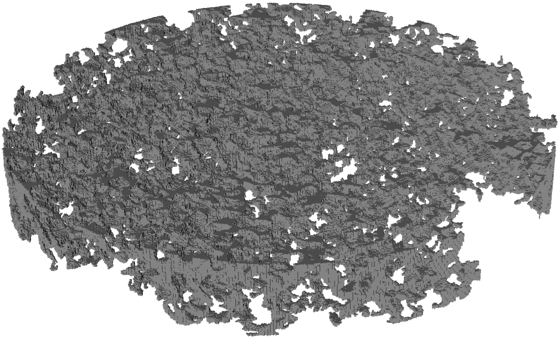
σ Interior Penalty parameter, $[\cdot]$ jumps and $\{\cdot\}$ averages across elements.

The solution u_n is exactly div-free (compatible), inspite of nonconformity.

This method easily generalisable to polytopic meshe...!

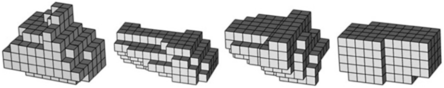
Fantastic Voyage: model reduction via cell agglomeration

[C, Dong, Georgoulis, Houston, Springer Briefs, 2017]



$\sim$ 3.2M cells/elements from voxels of a CT scan of bone scaffold

Use general polyhedral element shapes $\sim$32k elements

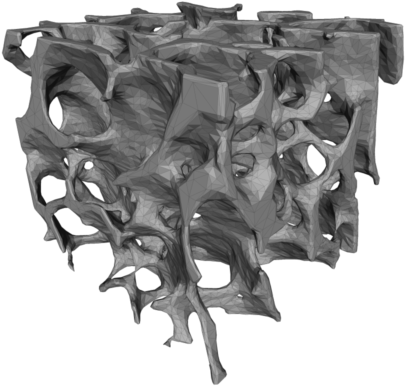


If higher resolution is required locally, use mesh adaptivity

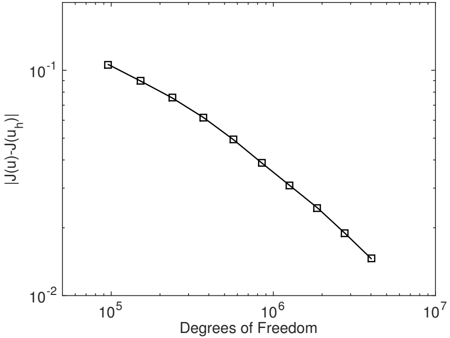
Goal oriented adaptivity on complicated domains

[C, Dong, Georgoulis, Houston, Springer Briefs, 2017]

Linear elastic analysis of a section of trabecular bone



- Model: 1,179,569 tetrahedral elements
- agglomerated to generate a coarse polytopic mesh of 8000 elements
- goal-oriented adaptive algorithm



Convergence of DWR error estimator of Young's modulus

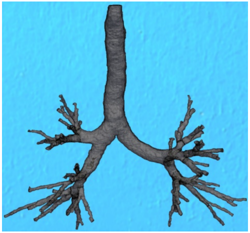
Mesh-based discretisations with general cells

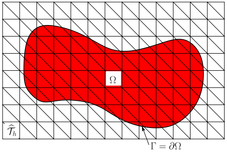
1. Nonstandard finite elementsmay be more suited to the problem
   $\rightarrow$ multiscale FEM, compatible discretisation methods

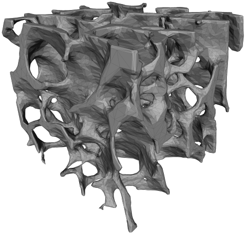
2. More general elemental shapes
   - Complex/complicated/curved/moving/multiphysics domains
   - Automatic mesh/order adaptivity

Typical configurations include

- curved (moving) geometries (eg. from CAD or level set descriptions from centrelines)
- multiscale geometries given as a fine pixelisation







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   $\rightarrow$ multiscale FEM, compatible discretisation methods

2. More general elemental shapes
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Main technologies developed including general mesh/order adaptivity:

- Virtual Element Method VEM [Beirao da Veiga, Brezzi, C, Manzini, Marini & Russo, M3AS, 2013]
- discontinuos Galerkin (dG) methods [C, Georgoulis & Houston, M3AS, 2014]

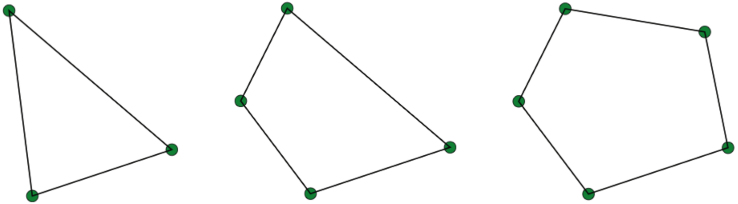
Common features: physical mesh elements robust with respect to mesh distortion, trivial & fully local adaptivity.

The Virtual Element Method (VEM) in a nutshell

[Beirao da Veiga, Brezzi, Cangiani, Manzini, Marini, & Russo, M3AS, 2013]

Reinterpret classical FE as instances of more general spaces (eg. conforming FE as generalised harmonic functions).

☞ As such, they yield the same element irrespective of the shape:



☞ Consistent and comforming discretisations on polygonal meshes.

☟ Disctrete space difficult to compute with eg. solutions of local PDEs).

The Virtual Element Method (VEM) in a nutshell

[Beirao da Veiga, Brezzi, Cangiani, Manzini, Marini, & Russo, M3AS, 2013]

- Use enriched spaces $V^\kappa = \mathcal{P}_p(\kappa) +$ 'virtual functions'
- Fix the DoF so that $\Pi : V^\kappa \to \mathcal{P}_p(\kappa)$ is computable just by accessing the DoF.
- Approximate the problem by only using directly accessible quantities.

$\Rightarrow$ conforming polynomial-like FEM on polygonal meshes.

Example: heat equation with manufactured solution

VEM adaptive algorithm:

$\tau = 0.000625$;

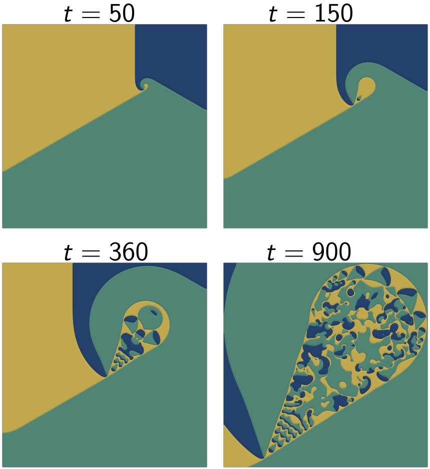
Refinement:
if indicator > 0.01,
every 5 steps

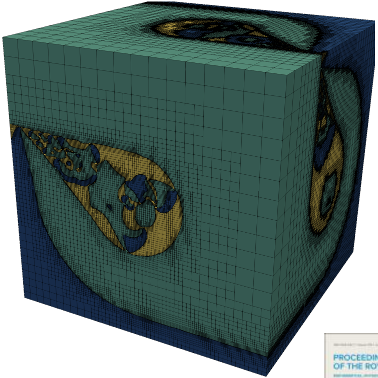
Coarsening:
if indicator < 0.0005,
every 20 steps.

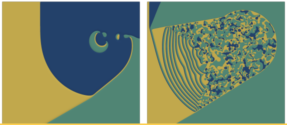
[C, georgoulis, Sutton, M3AS, 2021]

Revealing new dynamical patterns

Lotka-Volterra cyclic competition of mutually exclusive species







[C., Georgoulis, Morozov, Sutton, Proc. Royal Soc. A., 2018]

Adaptivity with general meshes

Mesh adaptive Virtual Element Method. [Sutton, PhD Thesis, Leicester, 2017]

A posteriori error bounds – a brief intro

$$
\begin{aligned}
-\Delta u =& f \quad \text{in } \Omega, \\
u =& 0, \quad \text{on } \partial\Omega.
\end{aligned}
$$

PDE stability via energy method: $\|\nabla u\| \le \|f\|_{H^{-1}(\Omega)}$
FEM: Find $u_h \in V_h \subset H_0^1(\Omega) : (\nabla u_h, \nabla v_h) = \langle f, v_h \rangle \quad \forall v_h \in V_h$.
We have, formally:

$$
\begin{aligned}
\|\nabla(u - u_h)\|^2_{L^2(\Omega)} \le& \|f + \Delta u_h\|^2_{H^{-1}(\Omega)} \\
=& C \sum_{\kappa \in \mathcal{T}} \eta_\kappa(u_h, f)
\end{aligned}
$$

This is a basic residual-based a posteriori error bound.

Residual-based a posteriori error estimation and adaptivity

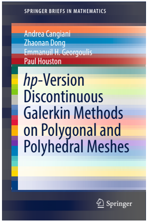
PDE stability + Galerkin orthogonality & Approximation error estimates

$\Downarrow$

Robust and efficient a posteriori[2] error estimation.

- A posteriori bounds used to drive automatic adaptive algorithms
- General meshes provide more flexible tool

  [Giani & Houston 2014, Collins & Houston 2016, C, Georgoulis & Sabawi 2017, C, Georgoulis, Pryer & Sutton 2017, C, Georgoulis & Sutton 2021, C, Georgoulis & Dong, 2022]



[C, Dong, Georgoulis & Houston 2017]

[2] A posteriori bounds only depend on computable quantities.

Typical posteriori error bound

Discontinuous Galerkin a posteriori error bound on general meshes

$$|||u - u_h|||^2 \leq C\Big(\sum_{\kappa\in\mathcal{T}} \big(\frac{h_\kappa^2}{p_\kappa^2}\|(f - \nabla_h(A\nabla_h u_h)\|_\kappa^2 + \frac{h_\kappa}{p_\kappa}\|[A\nabla u_h]\|_{\partial\kappa\cap\Gamma_{\mathrm{int}}}^2$$

$$\frac{h_\kappa}{p_\kappa}\|[\mathrm{t}\cdot\nabla u_h]\|_{\partial\kappa}^2 + \|\sigma^{1/2}[u_h]\|_{\partial\kappa}^2\big)\Big),$$

Typical tools:

Trace-inverse estimate

Given $p \in \mathbb{N}$, for each $\kappa \in \mathcal{T}$ and $v \in \mathcal{P}_p(\kappa)$,

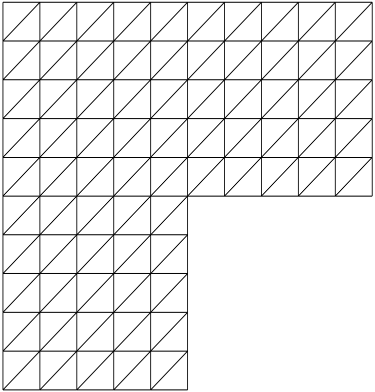
$$\|v\|_{\partial\kappa}^2 \leq C_{sh}\frac{(p+1)(p+d)}{h_\kappa}\|v\|_\kappa^2$$

Mesh adaptivity

[C., Dong &Georgoulis, 2022]

$$-\nabla \cdot (a\nabla u) = f \text{ with } a = 1 \times I_{2\times 2} \text{ on } \Omega := (-1,1)^2 \setminus (0,1) \times (-1,0),$$

$$u = r^{2/3}\sin(2\psi/3) + \exp(-1000((x-0.5)^2 + (y-0.25)^2)) + \exp(-1000((x-0.5)^2 + (y-0.75)^2))$$



Initial mesh, $p \equiv 3$

Mesh adaptivity

[C., Dong &Georgoulis, 2022]

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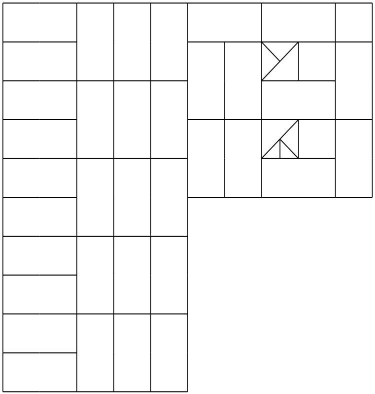

Adaptive mesh, $p \equiv 3$

Coarsening by agglomeration of neighbours with large tangential+normal jump residuals

Mesh adaptivity

[C., Dong &Georgoulis, 2022]

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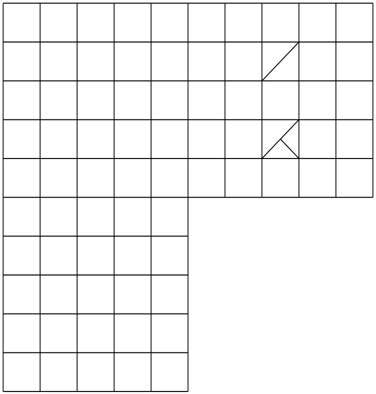

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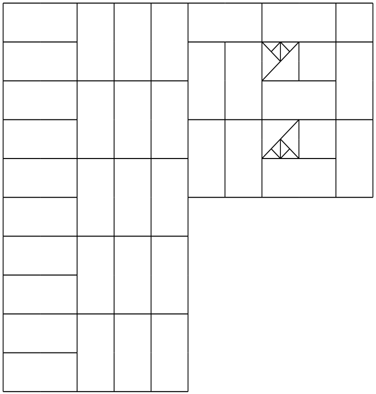

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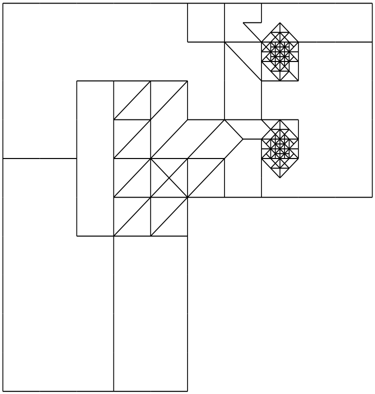

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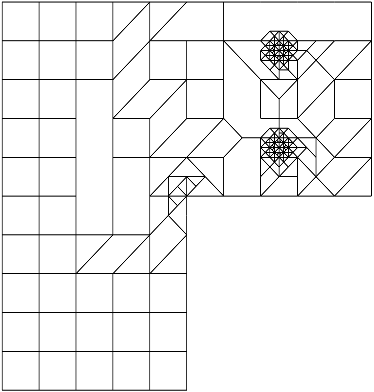

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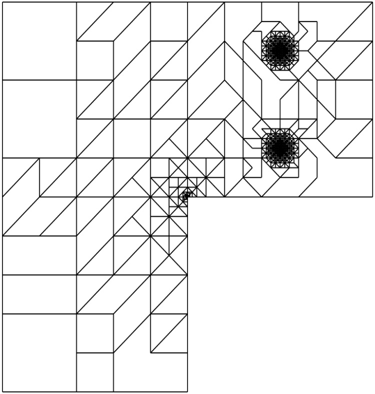

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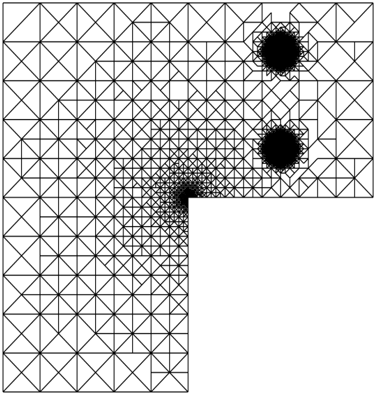

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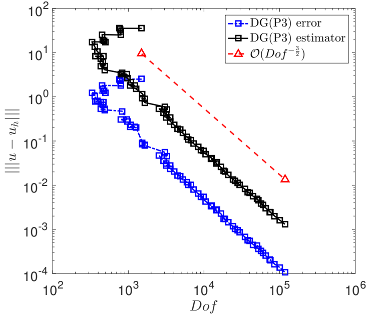
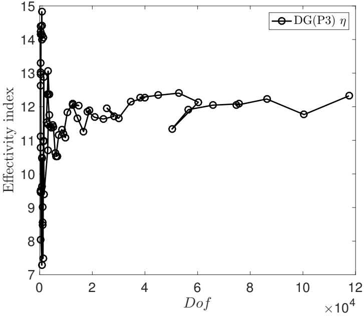
Convergence hystory and effectivity

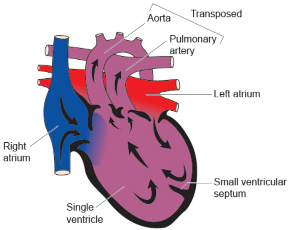
[C., Dong & Georgoulis, 2022]

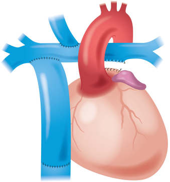




Univentricular heart: the Fontan circulation

Targeting poor long-term prognosis of new borns with functionally univentricular hearts.





[Corno et al., Frontiers in Pediatrics, 2019]

Fontan circulation ($\sim$1970) revolutionised the treatment of patients with "functionally" uni-ventricular hearts, previously considered inoperable.

Model of Fontan circulation

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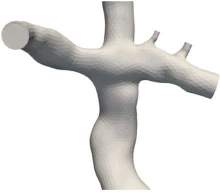

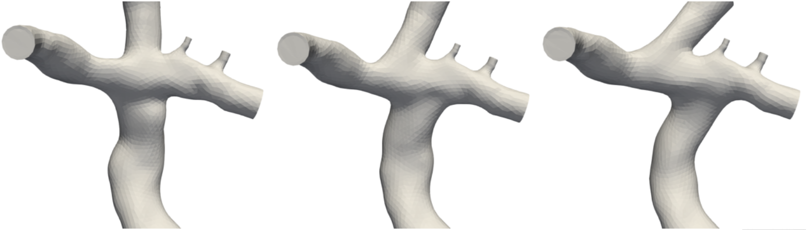

Model of Fontan circulation

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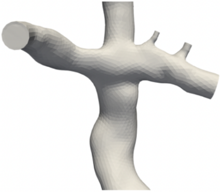
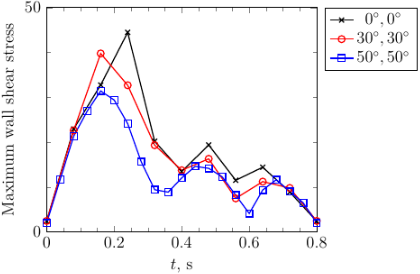
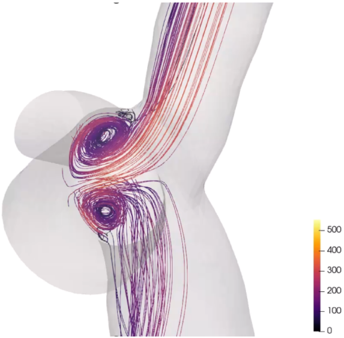
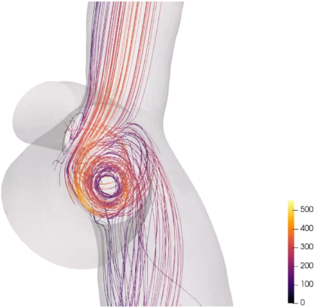




Simulations of Fontan circulation

Navier-Stokes with Robin b.c. by Zakhary Crowson using AptoFEM (Nottingham)





Cost of assembly of polyhedral FEM

GPU-accelerated stiffness matrix assembly [Dong, Georgoulis, Kappas, 2020].

(Times for a Nvidia P100 Graphical Processing Unit)

p	1	2	3	4	5
♯ elements	8,388,608	2,097,152	524,288	131,072	32,768
♯ DoFs	33.5M	20.1M	10.4M	4.6M	1.8M
kernels only (sec)	1.0s	3.5s	5.6s	7.1s	7.9s

Challenges & connections to other disciplines

Computational modelling of complex processes (biomedical): robustness, compatibility, and complexity reduction

- Compatible discretisations preserving geometry, conservation properties, symmetries, monotonicity,. . .
- Adaptive/automatic resolution, *eg.* of sharp solution features
- Parameters estimation, inverse problems, uncertainty quantification

Requires:

- Skillful knowledge of the physical/biological problem
- Deep mathematical analysis
- Development of HPC algorithms