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computational mathematics

# **Composite Finite Elements**

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## Introductory Example: Numerical Modelling of Trabecular Bones

Trabecluar Bone is the material microstructure of vertebral bodies.



Affected by osteoporosis by elderly humans.

3.79 millions osteoporotic fractures in Europe in 2000

Direct cost: 31.7 billion Euros.Goal: Reliable numerical simulation. Numerical challenge: Model contains very different scales Conventional Finite Elements need a huge number of degrees of freedom for the fine scale resolution.

Accuracy requirements are moderate.

Linearized Elasticity

Find  $u \in \mathbf{H}_{D}^{1}(\Omega)$  such that

$$\int_{\Omega} \mathbb{L}\varepsilon(u) : \varepsilon(v) = \int_{\Omega} fv \qquad \forall v \in \mathbf{H}_{D}^{1}(\Omega),$$

where

 $\varepsilon(u)$  is the symmetric strain tensor

$$\varepsilon(u) := \frac{1}{2} (\nabla u + (\nabla u)^{\mathsf{T}})$$

 $\mathbb{L}\varepsilon$  is the stress tensor

$$\sigma = \mathbb{L}\varepsilon = 2\mu\varepsilon + \lambda \operatorname{trace}(\varepsilon) \operatorname{Id}$$
.

The Lamé coefficients  $\mu$ ,  $\lambda$  have discontinuities at the trabeculae boundaries.

Boundary value problems with multiple scales

Goal: Flexible and adaptive modeling of problems with different scales such as:

- scales in the physical geometry
- scales in the data
- scales introduced by singular perturbations



von Mises stresses in porcine trabecular bone





Diffusion problem in heterogeneous media

Oscillatory solution of a non-linear Helmholtz equation

#### Model Problems

a) Poisson-type scalar elliptic equations.

 $\Omega \subset \mathbb{R}^d$  : bounded Lipschitz domain with boundary  $\Gamma = \partial \Omega$ ,

 $\mathcal{H}=(\omega_i)_{i=1}^q$  : disjoint inclusions in  $\Omega$ ,

 $\gamma = igcup_{i=1}^q \partial \omega_i$  :skeleton of the inclusions,

 $a \in L^{\infty}(\Omega)$ : diffusion coefficients $orall \omega \in \mathcal{H}: a|_{\omega} = a_{\omega} \in \mathbb{R}_{>0}$ 





### Continuous Problem:

Find  $u \in H^1_D(\Omega)$  such that

$$\int_{\Omega} \langle a \nabla u, \nabla v \rangle = \int_{\Omega} f v \qquad \forall v \in H_D^1(\Omega) \,.$$

Number of inclusions is huge and cannot be resolved by finite elements.

Goal: Define low-dimensional finite element spaces in a hierarchical way.

b) Stokes equation.

$$\begin{array}{rl} -\Delta \mathbf{u} & +\nabla p &= \mathbf{f} \\ \operatorname{div} \mathbf{u} & &= \mathbf{0} \end{array}$$

Boundary conditions:

with the stress tensor  $\sigma(\mathbf{u},p) = 2\varepsilon(\mathbf{u}) - p\mathbf{I}$ .

Sobolev spaces for velocity:

$$\mathbf{H}_{D}^{1}\left(\Omega
ight) := \left\{ \mathbf{u} \in \mathbf{H}^{1}\left(\Omega
ight) : \mathbf{u} = \mathbf{0} \quad \text{ on } \mathsf{\Gamma}_{D} 
ight\},$$
  
 $\mathbf{H}_{\mathsf{slip}}^{1}\left(\Omega
ight) := \left\{ \mathbf{u} \in \mathbf{H}^{1}\left(\Omega
ight) : \langle \mathbf{u}, \mathbf{n} 
angle = \mathbf{0} \quad \text{ on } \mathsf{\Gamma}_{\mathsf{slip}} 
ight\}.$ 

c) Highly indefinite Helmholtz equation.

Find  $u \in H^1(\Omega)$  such that

$$\int_{\Omega} \left( \langle \nabla u, \nabla \overline{v} \rangle - k^2 u \overline{v} \right) + \mathsf{i} \, k \int_{\partial \Omega} u \overline{v} = \int_{\Omega} f \overline{v} \qquad \forall v \in H^1(\Omega) \,.$$

The solutions become highly oscillatory for large wave numbers  $k \ge k_0 > 0$ .

**Composite Finite Elements** 

Concept:

- a. Introduce *dependent* nodes in vicinity of critical regions, i.e., boundary of the domain and/or of the inclusions.
- b. Define the values in the *dependent* nodes via a suitable extrapolation operator which reflects the characteristic behavior of the solution.
- c. The number and location of the *dependent* nodes are determined via an a-posteriori error estimator.

### Construction of Two-Scale Discretization I

- $\mathcal{G}_H$ : Overlapping finite element mesh determining the degrees of freedoms. The mesh width H is related to the desired accuracy.
- $\mathcal{G}_{H,h}$ : Finite element mesh which arises by refining recursively all simplices which overlap the boundary of the domain and/or the inclusions. The mesh width which characterizes the boundary resolution is h.
- $\mathcal{G}_{H,h}^{dep} \subset \mathcal{G}_{H,h}$ : Simplices which are generated by the boundary resolution.
- $\mathcal{G}_{H,h}^{dof} := \mathcal{G}_{H,h} \setminus \mathcal{G}_{H,h}^{dep}$ : Simplices which have a proper distance to the boundary.

Construction of Two-Scale Discretization II

 $\Theta_{H,h}$  : Total set of nodal points in the two-scale mesh  $\mathcal{G}_{H,h}$ 

 $\Theta_{H,h}^{dep}$ : Set of *dependent* nodes in the vicinity of the critical regions.

 $\Theta_{H,h}^{\mathsf{dof}}$  : Set of degrees of freedom.



For  $x \in \Theta_{H,h}^{dep}$ , let  $x^{\Gamma}$  denote a nearest point on the boundary/interface and let  $\Delta_x$  denote a nearest simplex in  $\mathcal{G}_{H,h}^{dof}$ .

Construction of Composite Finite Element Spaces:

a) Poisson-type problem with Neumann boundary conditions

Space of standard finite elements at proper distance to the boundary/interface is defined by

$$\begin{split} \Omega^{\mathsf{dof}}_{H,h} &:= \mathsf{int} \bigcup_{\tau \in \mathcal{G}^{\mathsf{dof}}_{H,h}} \tau. \\ S^{\mathsf{dof}}_{H,h} &:= \left\{ u \in C^{\mathsf{0}}\left(\Omega^{\mathsf{dof}}_{H,h}\right) \mid \forall \tau \in \mathcal{G}^{\mathsf{dof}}_{H,h} : u|_{\tau} \in \mathbb{P}_{1} \right\}. \end{split}$$

Extrapolation Operator:

Let  $u \in S_{H,h}^{\mathsf{dof}}$ .

• For nodal points  $x\in \Theta_{H,h}$ , the extrapolation operator is given by

$$\left(\mathcal{E}_{N}u
ight)\left(x
ight):=\left\{egin{array}{ll} u\left(x
ight) & x\in\Theta_{H,h}^{\mathsf{dof}},\ u_{\Delta_{x}}\left(x
ight) & x\in\Theta_{H,h}^{\mathsf{dep}}, \end{array}
ight.$$

where  $u_{\Delta x}$  is the affine extension of the restriction  $u|_{\Delta x}$  to  $\mathbb{R}^d$ .

 For x ∈ Ω, the extrapolation operator is the piecewise affine interpolation of the nodal values

$$\mathcal{E}_N u := (\mathcal{I}\mathbf{u})|_{\Omega}, \quad \text{where } \mathbf{u} := ((\mathcal{E}_N u)(x))_{x \in \Theta_{H,h}}$$

The space of composite finite elements is given by, locally, extending standard finite element functions from the interior to a near-boundary zone

$$S_{H,h} := \mathcal{E}_N S_{H,h}^{\mathsf{dof}}.$$

The basis functions are

- as for standard finite elements in the interior
- "smeared" from the interior to the boundary in a near-boundary zone.
- The system matrix is assembled by standard finite element technology while the supports of the modified basis functions are slightly increased leading to a slightly increased sparsity pattern.

### b) Poisson-type problem with Dirichlet boundary conditions

The concept for the construction is as for the natural boundary conditions while the definition extrapolation operator employs a suitable weight.

• For nodal points  $x \in \Theta_{H,h}$ , the extrapolation operator is given by

$$\left(\mathcal{E}_{D}u\right)(x) := \begin{cases} u(x) & x \in \Theta_{H,h}^{\mathsf{dof}}, \\ u_{\Delta_{x}}(x) - u_{\Delta_{x}}\left(x^{\mathsf{\Gamma}}\right) & x \in \Theta_{H,h}^{\mathsf{dep}}. \end{cases}$$

• For  $x \in \Omega$ , the extrapolation operator is the piecewise affine interpolation of the nodal values

$$\mathcal{E}_D u := (\mathcal{I}\mathbf{u})|_{\Omega}, \quad \text{where } \mathbf{u} := ((\mathcal{E}_D u)(x))_{x \in \Theta_{H,h}}.$$

#### c) Poisson-type problem with discontinuous coefficients

Let  $\gamma$  denote the interfaces between the inclusions. For a dependent node  $x \in \Theta_{H,h}^{dep}$ , let  $x^{\gamma} \in \gamma$  denote a nearest interface point and let  $\Delta_x^{I}$ ,  $\Delta_x^{II}$  denote nearest simplices on each side of the interface. We define

$$\left(\mathcal{E}_{\mathsf{jump}}u
ight)(x):=\left(\mathcal{E}_{N}u
ight)(x)-\left(\mathcal{E}_{N}u
ight)(x^{\gamma})+c^{\gamma},$$

where  $c_x^{\rm I},\,c_x^{\rm II}$  satisfy





If nearest simplices  $\Delta_x^{I}$ ,  $\Delta_x^{II}$  on different sides of  $\gamma$  do **not** exist because the inclusions are **too** small, the construction can be generalized to a multiscale agglomeration approach (work in progress).

If there is a huge number of small holes as in porous media the definition of the values in the dependent points should be done by solving local problems in a hierarchical way (see S., Warnke)





Basis for Neumann bc

Basis for Dirichlet bc



Basis for problems with discontinuous coefficients

## d) Lamé Equations for Problems in Linear Elasticity

The extension operator for problems in elasticity with *mixed boundary conditions* is defined as the componentwise application of the (previous) extension operators for Poisson-type problems.

## e) <u>Stokes Problem</u>

We consider the mini-element  $(S^{1,0} \oplus B)^d \times (S^{1,0} \cap L^2_0(\Omega))$ . The linear part of the velocity field  $\mathbf{u} \in (S^{1,0} \oplus B)^d$  is denoted by  $\mathbf{u}^{\text{lin}}$ .

Dirichlet boundary conditions: The extension operator  $\mathcal{E}_D$  is applied componentwise to the linear part of **u** to define values of the velocity in the dependent nodes.

Slip boundary conditions: The normal component is extended as in the case of Dirichlet boundary conditions while the tangential part is extended as for Neumann boundary conditions

$$\left( \mathcal{E}_{\mathsf{slip}} \mathbf{u} \right) (x) := \begin{cases} \mathbf{u} (x) & x \in \Theta_{H,h}^{\mathsf{dof}} \\ (\mathcal{E}_N \mathbf{u}) (x) - (\mathcal{E}_N \mathbf{u} (x))_{\mathbf{n} \left( x^{\Gamma} \right)} + (\mathcal{E}_D \mathbf{u} (x))_{\mathbf{n} \left( x^{\Gamma} \right)} & x \in \Theta_{H,h}^{\mathsf{dep}}. \end{cases}$$

### A Priori Analysis for Problems in Linear Elasticity

The composite finite element space for Dirichlet boundary conditions is nonconforming  $\mathbf{S}^{CFE} \not\subset \mathbf{H}_D^1(\Omega)$ .

**Theorem 1.** [Rech, Smolianski, S., NuMath] Let  $h \sim H^{3/2}$ . Then, the bilinearform  $a(\cdot, \cdot)$  is coercive on  $\mathbf{S}^{CFE} \subset \mathbf{H}_D^1(\Omega)$ , i.e., there exists  $\gamma > 0$  such that

$$a(u, u) \ge \gamma ||u||_{H^1(\Omega)}^2 \qquad \forall u \in \mathbf{S}^{\mathsf{CFE}}.$$

In particular, the Galerkin discretization has a unique solution.

**Theorem 2.** Let  $u \in H^1_D(\Omega) \cap H^{1+s}(\Omega)$ ,  $0 \le s \le 1$ . Suppose that the following conditions are satisfied

$$|\tau \cap \mathsf{\Gamma}| \le Ch_{\tau} \qquad \forall \tau \in \mathcal{G}_H$$

and  $h \leq H^{3/2}$ . Then, the Galerkin solution  $u_S \in \mathbf{S}^{\mathsf{CFE}}$  exists and fulfills for sufficiently small H

$$||u - u_S||_{m,\Omega} \le CH^{1+s-m} ||u||_{H^{1+s}(\Omega)},$$

for m = 0, 1 and C is independent of H and h.

**Proof.** M. Rech, thesis, 2006 and Rech, Smolianski, S., NuMath, 2006.

#### A Posteriori Error Estimation

The accuracy in the *approximation* of the Dirichlet boundary conditions can be controlled by an a-posteriori error estimator which takes into account the effect of approximate Dirichlet boundary conditions.

The error estimator consists of three terms. For any  $v \in H^1(\Omega)$ , we set

$$egin{aligned} &m_0^2\left(v
ight) \coloneqq \inf_{ ilde{v}\in H_D^1(\Omega)} a\left(v- ilde{v},v- ilde{v}
ight), \ &m_d^2\left(v,y^\star
ight) \coloneqq \int_\Omega \left(arepsilon\left(v
ight)-\mathbb{L}^{-1}y^\star
ight) arepsilon\left(\mathbb{L}arepsilon\left(v
ight)-y^\star
ight), \ &m_f^2\left(y^\star
ight) \coloneqq \| ext{div}\,y^\star+f\|_{L^2(\Omega)}. \end{aligned}$$

**Theorem 3.** The error of the nonconforming approximation  $v \in \mathbf{S}^{CFE}$  of the exact solution u can be estimated by

$$a (u - v, u - v)^{1/2} \le 2m_0 (v) + m_d (v, y^*) + C_\Omega m_f (y^*) \qquad \forall y^* \in H(\Omega, \operatorname{div}),$$
(1)

where  $C_{\Omega}$  is the constant in Friedrichs' inequality for the domain  $\Omega$ , i.e.,

$$C_{\Omega} := \sup_{w \in H^1_D(\Omega) \setminus \{0\}} \frac{\|w\|_{L^2(\Omega)}}{\|\nabla w\|_{L^2(\Omega)}}.$$

## Numerical Experiments

### Convergence Rates for the Galerkin Solution

 $\Omega = (-1,1)^2$  with a non-aligned rotated overlapping mesh.

level	dof	error one-scale CFE	$rac{error(\ell{-}1)}{error(\ell)}$	error <b>two-scale</b> CFE	$rac{error(\ell-1)}{error(\ell)}$
3	162	0.34297		0.24245	
4	834	0.18394	1.865	0.12183	1.990
5	3738	0.12994	1.416	0.05171	2.356
6	15786	0.09284	1.340	0.02155	2.340
7	64626	0.06402	1.450	0.00897	2.402

## A-Posteriori Error Estimators

# Effectivity Index

$$eff := \frac{\text{estimated energy error}}{\text{energy error}}.$$

level	dof	energy error	$\left  rac{error(\ell - 1)}{error(\ell)}  ight $	estimated error	effectivity index
3	243	0.234		1.345	5.74
4	1251	0.110	2.127	0.692	6.23
5	5607	0.0486	2.263	0.406	8.36
6	23679	0.0165	2.945	0.173	10.46

Analysis for Stokes Flow

Find  $(\mathbf{u},p)\in\mathbf{H}_{0}^{1}\left(\Omega
ight) imes L_{0}^{2}\left(\Omega
ight)$  such that

$$\begin{array}{rcl} a\left(\mathbf{u},\mathbf{v}\right)+b\left(\mathbf{v},p\right) &=& \left(\mathbf{f},\mathbf{v}\right) \\ b\left(\mathbf{u},q\right) &=& \mathbf{0} \end{array} \quad \forall \left(\mathbf{v},p\right) \in \mathbf{H}_{0}^{1}\left(\Omega\right) \times L_{0}^{2}\left(\Omega\right), \end{array}$$

where

#### Finite element approximation

Find  $(\mathbf{u}, p) \in \mathbf{X}_H \times M_H$  such that

$$\begin{array}{rcl} a\left(\mathbf{u},\mathbf{v}\right)+b\left(\mathbf{v},p\right) &=& \left(\mathbf{f},\mathbf{v}\right) \\ b\left(\mathbf{u},q\right) &=& \mathbf{0} \end{array} \quad \forall \left(\mathbf{v},p\right) \in \mathbf{X}_{H} \times M_{H}, \end{array}$$

where  $(\mathbf{X}_H, M_H)$  is the classical mini-element space, i.e.,

 $X_H$ : pw. linear functions enriched by cubic bubble functions

 $M_H$ : continuous, pw linear functions with integral mean zero.

**Classical Convergence Results** 

- Coercivity:  $\forall \mathbf{u}, \mathbf{v} \in \mathbf{X}_H$   $a(\mathbf{u}, \mathbf{u}) \geq \alpha \|\mathbf{u}\|_{\mathbf{H}^1(\Omega)}^2$
- Stability:

$$\inf_{p_{H}\in M_{H}}\sup_{\mathbf{v}_{H}\in\mathbf{X}_{H}\setminus\{0\}}\frac{b\left(\mathbf{v}_{H},p_{H}\right)}{\|\mathbf{v}_{H}\|_{\mathbf{H}^{1}(\Omega)}\|p_{H}\|_{L^{2}(\Omega)}}\geq\beta>0.$$

• Regularity:  $(\mathbf{u}, p) \in \mathbf{H}^{1+r}(\Omega) \times \mathbf{H}^{r}(\Omega)$  for some  $0 < r \leq 2$ .

Then: 
$$\|\mathbf{u} - \mathbf{u}_H\|_{\mathbf{H}^1(\Omega)} + \|p - p_H\|_{L^2(\Omega)} \le C_{\mathbf{f}} H^r$$
.

For complicated domains, composite finite elements violate the boundary conditions.

This leads to a *non-conforming method*:

 $\mathbf{X}_H \times \mathbf{M}_H \subsetneq \mathbf{H}_0^1(\Omega) \times L_0^2(\Omega)$  but  $\mathbf{X}_H \times \mathbf{M}_H \subset \mathbf{H}^1(\Omega) \times L^2(\Omega)$ .

Then:  $\|\mathbf{u} - \mathbf{u}_H\|_{\mathbf{H}^1(\Omega)} + \|p - p_H\|_{L^2(\Omega)} \le C_{\mathbf{f}} \left( H^r + \sup_{\mathbf{v}_H \in \mathbf{X}_H \setminus \{0\}} \frac{\|\mathbf{v}_H\|_{\mathbf{L}^2(\partial\Omega)}}{\|\mathbf{v}_H\|_{\mathbf{H}^1(\Omega)}} \right).$ 

Model Problem: Domain which contains small holes.



Most Naive Approach: Holes are neglected (due to limited computer capacity) and a quasi-uniform mesh is employed.



Left-top: Quasi-uniform mesh. Right-top: Absolute velocity error.

Left bottom: Numerical solution on quasi-uniform mesh. Right-bottom: Exact solution

Resolving the holes by an adaptive mesh requires 8 - 10 times more nodal points.



Left-top: Resolving adaptive mesh. Right-top: Absolute velocity error. Left bottom: Numerical solution on resolving mesh. Right-bottom: Exact solution Composite Mini Element. (Number of unknowns is comparable as for quasiuniform mesh)



Left-top: CME mesh. Right-top: Absolute velocity error.

Left bottom: Numerical solution on CME mesh. Right-bottom: Exact solution

Convergence Results:

**Theorem 4.** [Stability, Peterseim/S. SIAM J. Numer. Anal.] The composite mini element space satisfies the inf-sup-condition

 $\inf_{p \in M_{H,h}^{\mathsf{CME}} \setminus \{0\}} \sup_{\mathbf{u} \in \mathbf{X}_{H,h}^{\mathsf{CME}} \setminus \{0\}} \frac{b(\mathbf{u}, p)}{\|p\|_{L^{2}(\Omega)} \|\mathbf{u}\|_{\mathbf{H}^{1}(\Omega)}} \geq \beta > 0.$ 

**Theorem 5.** [Approximation Property, Peterseim/S. SIAM J. Numer. Anal.] The composite mini element space satisfies the standard approximation property already on the non-resolved scales.

$$\inf_{\mathbf{v}\in\mathbf{X}_{H,h}^{\mathsf{CME}}} \|\mathbf{u}-\mathbf{v}\|_{\mathbf{H}^{1}(\Omega)} + \inf_{q\in M_{H,h}^{\mathsf{CME}}} \|p-q\|_{L^{2}(\Omega)} \lesssim H\left(\|\mathbf{u}\|_{\mathbf{H}^{2}(\Omega)} + \|p\|_{H^{1}(\Omega)}\right).$$

**Theorem 6.** The discretization with the composite mini element has a unique solution  $(\mathbf{u}_{H,h}, p_{H,h})$ .

If 
$$(\mathbf{u}, p) \in \mathbf{H}^{1+r}(\Omega) \times H^r(\Omega)$$
 for some  $r \in \left]\frac{1}{2}, 1\right]$  then  
 $\left\|\mathbf{u} - \mathbf{u}_{H,h}\right\|_{\mathbf{H}^1(\Omega)} + \left\|p - p_{H,h}\right\|_{L^2(\Omega)} \lesssim (H^r + \rho_{\mathsf{nc}}(H,h)) \left\|\mathbf{f}\right\|_{\mathbf{H}^{r-1}(\Omega)},$ 

with the measure of non-conformity

$$\rho_{\mathsf{nc}}(H,h) := \sup_{\mathbf{v}_{H,h} \in \mathbf{X}_{H,h}^{\mathsf{CME}} \setminus \{\mathbf{0}\}} \frac{\left\| \mathbf{v}_{H,h} \right\|_{L^{2}(\partial \Omega)}}{\left\| \mathbf{v}_{H,h} \right\|_{H^{1}(\Omega)}} \lesssim \sqrt{H} \max_{\substack{\tau \in \mathcal{G}^{\mathsf{dof}} \ t \in \mathcal{G}^{\mathsf{slave}}(\tau) \\ t \cap \partial \Omega \neq \emptyset}} \frac{\mathsf{diam} t}{\mathsf{diam} \tau}.$$

If the small and coarse scales h and H satisfy  $h \sim H^{r+1/2}$ , the asymptotic convergence rates **already** hold on the coarse scales.