Finite element methods, FreeFEM, and Multiscale Problems

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MATHerials

Weak formulation of PDEs

Consider a second order PDE

$$\begin{cases} -\Delta u(x) = f(x) \text{ for all } x \in \Omega, \\ u(x) = 0 \text{ for all } x \in \partial\Omega. \end{cases}$$

$(\Omega \subset \mathbb{R}^d,\ f \in L^2(\Omega))$

Strong $\to$ weak/variational formulation (pointwise $\to$ volume):

1. Multiply by a test function $\varphi \in \mathcal{C}_0^\infty(\Omega)$,
2. Integrate, use integration by parts.

$$\begin{aligned} \int_\Omega f\varphi = \int_\Omega \varphi(-\Delta u) &= -\int_{\partial\Omega} \varphi\vec{n} \cdot \nabla u + \int_\Omega \nabla\varphi \cdot \nabla u \\ &= \int_\Omega \nabla\varphi \cdot \nabla u \end{aligned}$$

Only first order derivatives, u and φ 'are in the same space.'

Weak formulation (ctd.)

Functional setting: find $u \in H_0^1(\Omega)$ such that

$$\forall\, v \in H_0^1(\Omega), \quad a(u, v) := \int_\Omega \nabla v \cdot \nabla u = \int_\Omega f\, v.$$

There is a unique u due to coercivity of a (Lax-Milgram).

Discrete approximation: solve the same problem on a finite-dimensional subspace V of $H_0^1(\Omega)$.

- This is called a Galerkin approximation.
- When $V = V_{\mathcal{T}}$ is associated to a mesh $\mathcal{T}$ of Ω, we have a finite element method.

Example: we will now solve $-\Delta u = 1 + y^2$ on the unit disk.

FreeFEM

Define the mesh

```
border bOmega(t=0, 2*pi) {x=cos(t);y=sin(t);label=1;} //unit
     disk; label is used later to set the boundary condition
int Nboundary = 20; //number of vertices on bOmega for our
    mesh
mesh T = buildmesh(bOmega(Nboundary)); //our mesh
```

Define the terms of the variational formulation

```
macro a(u,v) (dx(u)*dx(v) + dy(u)*dy(v)) //the macro is
    inserted whenever we type a(.,.)
func f=1+y^2; //the right-hand side function of our problem
```

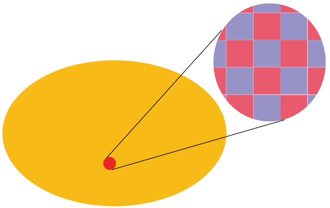
Define the Galerkin approximation & solve

```
fespace V(T, P1); //piecewise affine elements on the mesh T
V u,v; //set the space for the trial function (u) and test
    function (v)
solve pb(u,v)=int2d(T)(a(u,v)) - int2d(T)(f*v) + on(1, u=0);
     //the Galerkin approximation is solved for u
```

Multiscale diffusion problem

We seek a numerical approximation of u^ε solution to

$$\begin{cases} -\mathrm{div}(A^\varepsilon \nabla u^\varepsilon)(x) = f(x) \text{ for all } x \in \Omega, \\ u(x) = 0 \text{ for all } x \in \partial\Omega. \end{cases}$$



A^ε varies on a very small scale ε

Weak formulation

Find $u^\varepsilon \in H^1_0(\Omega)$ such that

$$\forall\, v \in H^1_0(\Omega), \quad a^\varepsilon(u^\varepsilon, v) := \int_\Omega \nabla v \cdot A^\varepsilon \nabla u^\varepsilon = \int_\Omega f\, v.$$

There is a unique solution if A^ε is coercive.

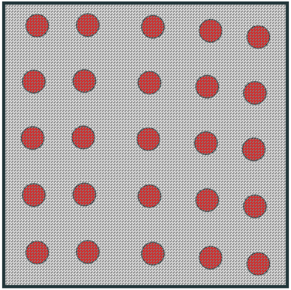
We cannot use a standard $\mathbb{P}_1$ method on a coarse mesh...

FEM with a microstructure

Example

$$-\operatorname{div}(A^\varepsilon \nabla u^\varepsilon) = 500$$

- ○ $A^\varepsilon = 1$
- ● $A^\varepsilon = 30$

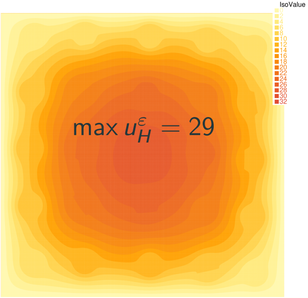


$\mathbb{P}_1$ **finite element method**

$V =$ continuous piecewise $\mathbb{P}_1$ functions on $\mathcal{T}$

Approximation with 10^6 degrees of freedom,

mesh size $\ll \varepsilon$



FEM with a microstructure

Example

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- ○ $A^\varepsilon = 1$
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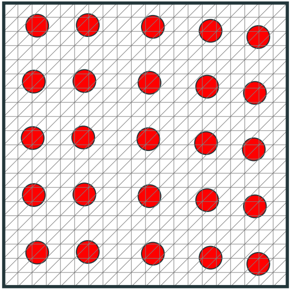
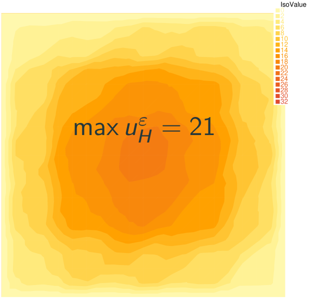


$\mathbb{P}_1$ finite element method

$V =$ continuous piecewise $\mathbb{P}_1$ functions on $\mathcal{T}$

Approximation with 441 degrees of freedom,

mesh size $\sim \varepsilon$



Example

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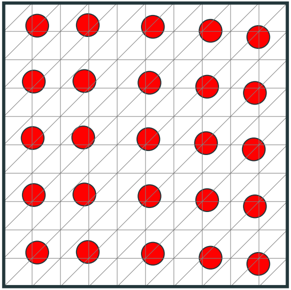
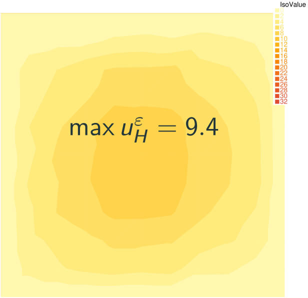


$\mathbb{P}_1$ finite element method

V = continuous piecewise $\mathbb{P}_1$ functions on $\mathcal{T}$

Approximation with 121 degrees of freedom,

mesh size $\geq \varepsilon$



FEM with a microstructure

Example

$$-\operatorname{div}(A^\varepsilon \nabla u^\varepsilon) = 500$$

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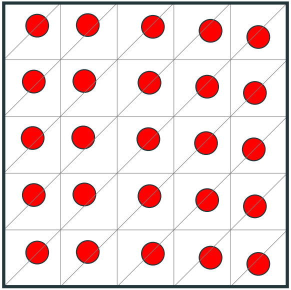
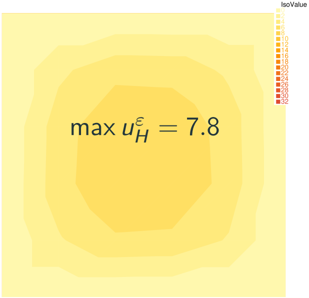


$\mathbb{P}_1$ finite element method

V = continuous piecewise $\mathbb{P}_1$ functions on $\mathcal{T}$

Approximation with 36 degrees of freedom,

mesh size $\gg \varepsilon$



Example

$$-\operatorname{div}(A^\varepsilon \nabla u^\varepsilon) = 500$$

- ○ $A^\varepsilon = 1$
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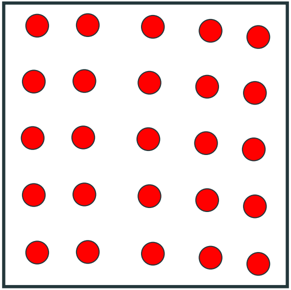
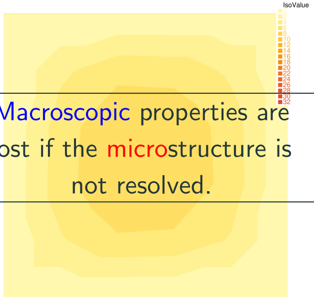


$\mathbb{P}_1$ finite element method

V = continuous piecewise $\mathbb{P}_1$ functions on $\mathcal{T}$



Macroscopic properties are lost if the microstructure is not resolved.

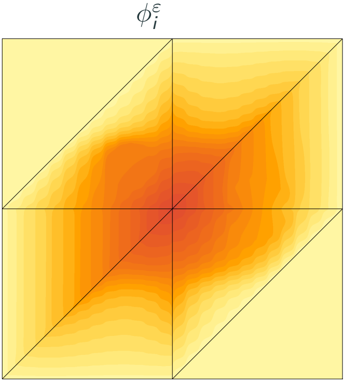
Numerical homogenization

Heterogeneous Multiscale Method (E and Engquist 2003), Local Orthogonal Decomposition (Målqvist and Peterseim 2014), we focus on the Multiscale Finite Element Method (MsFEM) (Hou and Wu 1997)

1. Offline stage: resolve the microstructure locally

Multiscale trial functions: $\forall\, K \in \mathcal{T}$,

$$\begin{cases} -\operatorname{div}(A^\varepsilon \nabla \phi_i^\varepsilon) = 0 & \text{in } K, \\ \phi_i^\varepsilon = \phi_i^{\mathbb{P}_1} & \text{on } \partial K. \end{cases}$$



2. Online stage: solve a coarse global problem

Find $u_{\mathcal{T}}^\varepsilon \in V_{\mathcal{T}}^\varepsilon = \operatorname{span}\{\phi_i^\varepsilon\}$ s.t. (Biezemans et al. 2022)

$$\forall\, v_{\mathcal{T}} \in V_{\mathcal{T}} \;:\quad a^\varepsilon\left(u_{\mathcal{T}}^\varepsilon, v_{\mathcal{T}}\right) = F(v_{\mathcal{T}})$$

Implementation of the MsFEM

We are not going to change FreeFEM's standard basis functions...

Link between $\phi_i^{\mathbb{P}_1}$ and ϕ_i^ε on $K \in \mathcal{T}$:

$$-\mathrm{div}\left(A^\varepsilon \nabla \left(\phi_i^\varepsilon - \phi_i^{\mathbb{P}_1}\right)\right) = \mathrm{div}\left(A^\varepsilon \nabla \phi_i^{\mathbb{P}_1}\right) = \sum_{\alpha=1}^{d} \left(\partial_\alpha \phi_i^{\mathbb{P}_1}\Big|_K \right) \mathrm{div}\left(A^\varepsilon e_\alpha\right).$$

Define $\chi_K^{\varepsilon,\alpha} \in H_0^1(K)$ by[1]

$$-\mathrm{div}\left(A^\varepsilon \nabla \chi_K^{\varepsilon,\alpha}\right) = \mathrm{div}\left(A^\varepsilon e_\alpha\right).$$

Then

$$\phi_i^\varepsilon = \phi_i^{\mathbb{P}_1} + \sum_{\alpha=1}^{d} \left(\partial_\alpha \phi_i^{\mathbb{P}_1}\Big|_K \right) \chi_K^{\varepsilon,\alpha} \quad \text{on } K.$$

[1] In principle, this problem does not even have to be solved with FreeFEM.

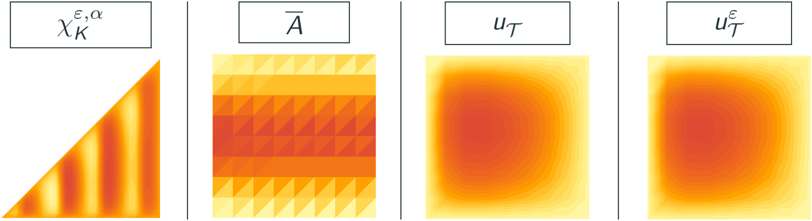
Effective PDE

$$\boxed{\text{Decoupling:} \qquad \phi_i^\varepsilon = \phi_i^{\mathbb{P}_1} + \sum_{K\in\mathcal{T}} \sum_{\alpha=1}^{d} \left(\partial_\alpha \phi_i^{\mathbb{P}_1}\right)\Big|_K \chi_K^{\varepsilon,\alpha}}$$

$$\begin{aligned}
a^\varepsilon\left(\phi_i^\varepsilon, \phi_j^{\mathbb{P}_1}\right) &= \sum_{K\in\mathcal{T}} \int_K \nabla \phi_j^{\mathbb{P}_1} \cdot A^\varepsilon \nabla \phi_i^\varepsilon \\
&= \sum_{K\in\mathcal{T}} \sum_{\alpha,\beta=1}^{d} \int_K \partial_\beta \phi_j^{\mathbb{P}_1} \, e_\beta \cdot A^\varepsilon \left(e_\alpha + \nabla \chi_K^{\varepsilon,\alpha}\right) \partial_\alpha \phi_i^{\mathbb{P}_1} \\
&= \sum_{K\in\mathcal{T}} \sum_{\alpha,\beta=1}^{d} \partial_\beta \phi_j^{\mathbb{P}_1}\Big|_K \left(\int_K e_\beta \cdot A^\varepsilon \left(e_\alpha + \nabla \chi_K^{\varepsilon,\alpha}\right)\right) \partial_\alpha \phi_i^{\mathbb{P}_1}\Big|_K \\
&= \sum_{K\in\mathcal{T}} |K| \left(\nabla \phi_j^{\mathbb{P}_1} \cdot \overline{A} \nabla \phi_i^{\mathbb{P}_1}\right)\Big|_K = \int_\Omega \nabla \phi_j^{\mathbb{P}_1} \, \overline{A} \nabla \phi_i^{\mathbb{P}_1}
\end{aligned}$$

$$\text{Effective matrix } \overline{A}_{\beta,\alpha}\Big|_K = \frac{1}{|K|} \int_K e_\beta \cdot A^\varepsilon \left(e_\alpha + \nabla \chi_K^{\varepsilon,\alpha}\right)$$

Non-intrusive MsFEM (Biezemans et al. 2022)



Example: Implement the MsFEM in FreeFEM with

$$A^{\varepsilon}(x, y) = (2 + \cos(2\pi y)) \left(1 + \frac{1}{4} \cos\left(\frac{2\pi x}{\varepsilon}\right)\right) \mathrm{Id}_2$$

MsFEM with FreeFEM

Define the microstructure

```
int Nmicro=8; //size of the microscale
real eps=1./Nmicro; //microscopic parameter
func nu=(2+cos(2*pi*y))*(1+0.25*cos(2*pi*x/eps)); //diffusion coefficient
macro aeps(u,v) (nu*dx(u)*dx(v) + nu*dy(u)*dy(v)) //EOM //volume term corresponding to the PDE
int Nresolve = 10*Nmicro; //determines the mesh size for the discretization of the microstructure
```

MsFEM with FreeFEM

Offline stage - initiation

```
real[int,int] chiX(T.nt,Nresolve^2); chiX=0; //to store chiX for all Ti
real[int,int] chiY(T.nt,Nresolve^2); chiY=0; //to store chiY for all Ti
fespace V0(T,P0); //piecewise constant elements;
V0 AbarXX, AbarYX, AbarXY, AbarYY; //coefficients of the effective diffusion matrix
macro aeff(u,v)  (dx(v)*AbarXX*dx(u) + dy(v)*AbarYX*dx(u) + dx(v)*AbarXY*dy(u) + dy(v)*AbarYY*dy(u) ) // EOM // volume term corresponding to the effective PDE
for (int i=0; i<T.nt; i++) {//loop over all triangles of T (their number is T.nt)
```

MsFEM with FreeFEM

Offline stage - build the local mesh

```
real x0=T[i][0].x, y0=T[i][0].y; //save vertex coordinates of the ith element of T
real x1=T[i][1].x, y1=T[i][1].y;
real x2=T[i][2].x, y2=T[i][2].y;
border T0(t=0,1) {x=x0*(1-t)+x1*t; y=y0*(1-t)+y1*t; label=1;}
border T1(t=0,1) {x=x1*(1-t)+x2*t; y=y1*(1-t)+y2*t; label=1;}
border T2(t=0,1) {x=x2*(1-t)+x0*t; y=y2*(1-t)+y0*t; label=1;}
mesh Ti = buildmesh(T0(Nresolve) + T1(Nresolve) + T2(Nresolve));
```

MsFEM with FreeFEM

Offline stage - local discrete problem

```
fespace Vi(Ti,P1); //P1 space on the fine scale mesh for the ith element of T
Vi uloc, vloc, uH, chiXi, chiYi; //solution and test functions in the space Vi
Vi uHx=x , uHy=y; //functions to define the right-hand side of the variational formulation
problem corrector(uloc,vloc) = int2d(Ti)(aeps(uloc,vloc)) - int2d(Ti)(aeps(uH,vloc)) + on(1, uloc=0);
uH=uHx; corrector; chiXi[]=uloc[]; chiX(i,:)=chiXi[];
uH=uHy; corrector; chiYi[]=uloc[]; chiY(i,:)=chiYi[];
```

MsFEM with FreeFEM

Offline stage - compute the effective matrix

```
    Vi phiX, phiY;
    phiX[]=uHx[]+chiXi[];
    phiY[]=uHy[]+chiYi[];
    AbarXX[][i]=int2d(Ti)(aeps(phiX,uHx))/Ti.measure;
    AbarYX[][i]=int2d(Ti)(aeps(phiX,uHy))/Ti.measure;
    AbarXY[][i]=int2d(Ti)(aeps(phiY,uHx))/Ti.measure;
    AbarYY[][i]=int2d(Ti)(aeps(phiY,uHy))/Ti.measure;
```

Effective matrix: $\overline{A}_{\beta,\alpha}\big|_K = \frac{1}{|K|}\int_K e_\beta \cdot A^\varepsilon \left(e_\alpha + \nabla\chi_K^{\varepsilon,\alpha}\right)$

Online stage

```
fespace V(T, P1); //piecewise affine elements on the mesh T
V u,v; //set the space for the trial function (u) and test
    function (v)
solve pb(u,v)=int2d(T)(aeff(u,v)) - int2d(T)(f*v) + on(1, u=
    0); //the Galerkin approximation is solved for u
```

MsFEM with FreeFEM

Reconstruction at the microscale

```
V0 xb=x, yb=y; //interpolation of the coordinate functions
    at the centroids of the mesh elements
V0 uP0=u; //interpolation of the global finite element
    solution at the centroids of the mesh elements
V0 udxP0=dx(u), udyP0=dy(u); //interpolation of the gradient
     of u at the centroids of the mesh elements
for (int i=0; i<T.nt; i++) {//loop over all triangles of T
    // ...construction of Ti for the ith element of T...
    fespace Vi(Ti,P1);
    Vi umicro;
    Vi phiX=x-xb[][i], phiY=y-yb[][i];
    phiX[]+=chiX(i,0:Vi.ndof-1); //last index is included in
     this syntax
    phiY[]+=chiY(i,0:Vi.ndof-1);
    umicro[]=uP0[][i];
    umicro[]+=udxP0[][i]*phiX[];
    umicro[]+=udyP0[][i]*phiY[];
}
```