

Computer lab Numerical Algorithms

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Problem sheet 1

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We consider the cell problem posed in the lecture: For a given (linear) profile u_H we want to compute a periodic correction u_h such that $-\operatorname{div}(a(u_H + u_h)) = 0$ and $\oint u_h \, dx = 0$. Using the periodicity assumptions the weak formulation is:

$$\int_Q a(x) \nabla u_h(x) \cdot \nabla \varphi_h(x) \, dx = - \int_Q a(x) \nabla u_H(x) \cdot \nabla \varphi_h(x) \, dx \quad \forall \varphi_h \in \mathcal{V}_h$$

For discretization we consider a triangulation \mathcal{T}_h and a corresponding set of finite element basis functions $\{\varphi_h^i\}_{i \in I}$. By writing $u_h = \sum_{j \in I} u_h^j \varphi_h^j$ and choosing basis functions as test functions in the weak formulation above we derive a linear system of equations $A \bar{u}_h = \bar{b}$ where

$$A_{ij} = a(\varphi_h^i, \varphi_h^j) = \int_Q a(x) \nabla \varphi_h^i(x) \cdot \nabla \varphi_h^j(x) \, dx, \quad b_i = (A \bar{u}_H)_i$$

The periodic boundary conditions will be enforced by modifying the stiffness matrix A and the right hand side \bar{b} .

We will start by assembling the stiffness matrix A which is usually done in the following way:

Assemblation of the stiffness matrix A

foreach triangle T **do**

foreach pair of basis functions φ_i, φ_j which have T in their support **do**

foreach quadrature point γ_T with weight ω_{γ_T} **do**

$A_{ij} += |T| * \omega_{\gamma_T} * a(T, \gamma_T, i, j)$

An implementation of this procedure can be seen in class `LinearFEOperator`. The function $a(T, \gamma_T, i, j)$ must now evaluate the integrand $a(x(\gamma_T)) \nabla \varphi_h^i(x(\gamma_T)) \cdot \nabla \varphi_h^j(x(\gamma_T))$ at the given quadrature point γ_T in T for basis functions φ_h^i and φ_h^j . It will be implemented in a separate class `IsoDiffusiveBilf`.

This class must be able to evaluate the diffusivity a at a given point. Therefore it has a member variable `TensorOrder0`. To allow for more general diffusivity terms later the class `TensorOrder0` is pure virtual and just defines that every derived class must supply

the required `evaluate` method. We will implement a derived class `BlobTensor` which realizes the following diffusivity:

$$a(x) = \psi_\varepsilon(\|x - m\|), \quad \text{where } \psi_\varepsilon(s) = -\frac{1}{\pi} \arctan\left(\frac{2s-1}{\varepsilon}\right) + \frac{1}{2}$$

The midpoint m and the “transition width” $\varepsilon \in (0.01, 0.5)$ should be selectable.

To take periodic boundary conditions into account we propose to first assemble the usual stiffness matrix A above and then perform modifications on A to reflect periodicity. This will be done by class `PeriodicBoundaryMask` derived from `BoundaryMask` (as is `DirichletBoundaryMask` which was used in problem 1).

In the constructor of this class a mapping needs to be generated which maps boundary nodes to their periodic counterparts. This could e.g. be realized using a vector of pairs of integers: `std::vector< SmallVector2<int> >`. Here one has to decide which nodes get eliminated by the periodic identification. Moreover the class should provide a method `apply` which collapses the matrix as discussed on problem sheet 1. To tackle the right hand side accordingly a method `collapse` should be implemented. Finally method `extend` is supposed to copy values at remaining boundary nodes to their eliminated counterparts.

So far the additional constraint $\int u_h dx = 0$ has not been accounted for. In the discrete setting the non uniqueness of solutions to the periodic cell problem will result in a rank deficiency of the resulting stiffness matrix. While in practice a CG method started from a feasible point \bar{u}_h might just iterate in the correct linear subspace we want to enforce this by additional projection steps. Therefore the constraint is discretized in the known manner:

$$\begin{aligned} 0 &= \int u_h dx = |Q|^{-1} \int_Q u_h 1 dx = |Q|^{-1} \sum_{i,j} u_h^i \int_Q \varphi_i \varphi_j dx \\ &\rightsquigarrow |Q|^{-1} \bar{u}_h^\top M \bar{1} = 0 \quad \text{where } M_{ij} = \int_Q \varphi_i \varphi_j dx \end{aligned}$$

That way $\tilde{n} := |Q|^{-1} M \bar{1}$ is orthogonal to every \bar{u}_h fulfilling the constraint. With a normalized normal vector $n := \tilde{n} / \|\tilde{n}\|$ the orthogonal projection of an arbitrary point x is given by $P(x) = x - (x \cdot n) n$. This projection may be performed after each step of a CG method as it does not affect the residual. To set up the normal vector n a mass matrix M can be generated analogously to the stiffness matrix by using the bilinear form `MassBilf`.

Tasks:

- Implement the scalar tensor `BlobTensor` derived from `TensorOrder0`
- Complete the class `IsoDiffusiveStiffBilf`
- For the class `PeriodicBoundaryMask` implement the constructor and methods `apply`, `collapse` and `extend`
- In the main function setup the right hand side from the given `Vector` u_H and perform the necessary periodic identification operations
- Implement `projectingCGapply` to perform a usual CG iteration with additional orthogonal projection along a supplied `Vector` `constr` ($= n$)