Draft on Dune-Fem-Functionals

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Abstract

This document is a draft about a new concept of DUNE-FEM based on functionals. DUNE-FEM is part of the Distributed and Unified Numerics Environment (DUNE) and is available from http://dune.mathematik.uni-freiburg.de/.

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1 Introduction

The overall goal of Dune-Fem and Dune-Fem-Functionals is the efficient numerical solution of PDE's. Assuming standard notation, the following elliptic PDE may serve as a sample problem.

Example 1.1 (Elliptic PDE in one dimension).

Let $\Omega \subset \mathbb{R}$ be a domain and $a, f : \Omega \to \mathbb{R}$ and $g : \partial\Omega \to \mathbb{R}$ be given functions. Find $u : \Omega \to \mathbb{R}$, such that

$$-\nabla \cdot (a\nabla u) = f \qquad in \Omega,$$

$$u = g \qquad on \partial\Omega.$$
(1.1)

$\textbf{Definition 1.2.} \ \textit{Weak formulation}$

Let H^1 and H^1_0 be given as usual and let H^1_g for $g \in H^1$ be defined as

$$H_q^1 := \{ v \in H^1 | v = w + g \text{ for } a w \in H_0^1 \}.$$

The weak formulation of problem (1.1) then reads as follows. Find $u \in H_g^1$, such that

$$\int_{\Omega} a\nabla u \nabla v \, dx = \int_{\Omega} f v \, dx \qquad \qquad for \ all \ v \in H_0^1. \tag{1.2}$$

The weak formulation (1.2) gives rise to the introduction of functionals and operators. A rigorous mathematical definition of these can be found in the next section. The following is only intended to give the basic idea.

Definition 1.3 (Operators and functionals).

The function f from he original problem 1.1 induces a functional

$$F: H_0^1 \to \mathbb{R}$$
$$v \mapsto F[v] := \int_{\Omega} fv \, dx.$$

Accordingly the function a from the original problem 1.1 induces an operator

$$A: H_g^1 \to H^{-1}$$
$$u \mapsto A(u),$$

where A(u) itself is a functional, defined by

$$A(u): H_0^1 \to \mathbb{R}$$

$$v \mapsto A(u)[v] := \int_{\Omega} a \nabla u \nabla v \, dx.$$

With these definitions at hand the weak formulation (1.2) can be rewritten in the following way.

Remark 1.4 (Variational formulation using functionals and operator). Let A and F be as in definition 1.3. The weak formulation (1.2) can be rewritten as follos. Find $u \in H_q^1$, such that

$$A(u)[v] = F[v] \qquad \qquad for \ all \ v \in H_0^1. \tag{1.3}$$

Our postulate is, that a wide range of interesting problems can be written in this form. For detailed examples of linear and nonlinear problems see section?.

2 Analytical concept

We start with an overview on the mathematical concept which is carried over to a corresponding programming concept. The following notations and definitions are required for the subsequent sections.

Definition 2.1 (Function and Functionspace).

Let $n, d \in \mathbb{N}^{\geq 1}$ be integers and $\Omega \subseteq \mathbb{R}^n$ a subset. A mapping $v : \Omega \to \mathbb{R}^d$ is called a function, the set

$$V := \{v : \Omega \to \mathbb{R}^d\}$$

is called a function space. If V is an \mathbb{R} -vector space, V is called a linear function space.

Definition 2.2 (Functional).

Let V be a function space. A map

$$F: V \to \mathbb{R},$$

$$v \mapsto F[v] \tag{2.1}$$

is called a Functional. If

$$F[\alpha v_1 + \beta v_2] = \alpha F[v_1] + \beta F[v_2]$$

holds for all $\alpha, \beta \in \mathbb{R}$ and all $v_1, v_2 \in V$, F is called a Linear Functional. The vector space

$$V' := \{F : V \to \mathbb{R} | F \text{ is a linear functional } \}$$
 (2.2)

is called the dual space of V.

Definition 2.3 (Constraint).

Let V be a linear function space, $M \in \mathbb{N}_{>0}$ and $\{F_1, ..., F_M\}$ a set of linear functionals on V. We define the corresponding vector of linear functionals C by

$$C: \{1, ..., M\} \times V \to \mathbb{R} \text{ with } (i, v) \mapsto C[i][v] := F_i[v].$$
 (2.3)

The condition:

$$C[i][v] = 0 \ \forall 1 \le i \le M \tag{2.4}$$

is called a Constraint for v.

In particular each linear functional implies a constraint.

Definition 2.4 (Linear Subspace).

Let V be a linear function space and $C[\cdot][\cdot] = 0$ a constraint on V. Then we call

$$V_C := \{ v \in V \mid C[i][v] = 0 \ \forall i \in \{1, ..., M\} \}$$
 (2.5)

a linear subspace of V with respect to C.

 V_C is a vector space itself, since the constraint functionals C[i] are linear. Typically, V_C becomes the space of test functions in our later problem.

Definition 2.5 (Affine space).

Let V be a function space, V_C a linear subspace and $g \in V$. Then we call

$$V_q := \{ v + g | v \in V_C \} \subset V \tag{2.6}$$

an affine space with respect to g and V_C .

In general, V_g is only a subset of V and not a subspace. It will be the space of solutions in our later problem.

Definition 2.6 (Operator).

Let V be a linear function space, $V_C \subset V$ a linear subspace, V'_C its dual and $V_g \subset V$ an affine space. Then we call

$$G: V_q \to V_C'$$
 (2.7)

an operator on V_q . If

$$G(\alpha v + \beta w) = \alpha G(v) + \beta G(w)$$

holds for all $\alpha, \beta \in \mathbb{R}$ and for all $v, w \in V_q$ the operator G is called linear.

In the subsequent sections, we are dealing with the following problem.

Problem 2.7. Sample problem

Let V be a linear space, $V_C \subset V$ a linear subspace, $F \in V'_C$ a functional and $V_g \subset V$ an affine space. Find $u \in V_g$, such that

$$G(u)[v] = F[v]$$
 for all $v \in V_C$.

In general, the functional F on the right hand side of our problem is linear. The (differential) operator G can be either linear or nonlinear.

3 Examples

3.1 Elliptic PDE

Let $\Omega \subset \mathbb{R}^d$ denote a polygonal bounded domain, $\mathcal{T}_H = \{T_1, ..., T_N\}$ a corresponding regular triangulation, $\mathcal{N}_H = \{x_1,, x_{\tilde{N}}\}$ the set of nodes and $\{\Phi_1,, \Phi_{\tilde{N}}\}$ the associated Lagrange basis of order 1. The (discrete) linear space of solutions is given by

$$V := \left\{ v_H \in C^0(\Omega) \middle| (v_H)_{|T} \in \mathbb{P}^1(T) \quad \forall T \in \mathcal{T}_H \right\}$$

and the linear subspace of testfunctions by $V_0 := V \cap H_0^1(\Omega)$. Now, let us consider the following discrete problem.

Problem 3.1.

For $g \in V$ find $u \in V$ with u = g on $\partial \Omega$ and

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \qquad \qquad \text{for all } v \in V_0.$$

(Note: V_0 can not be replaced by V).

Putting this into the general framework above, we define the (linear) functional $F:V_0\to\mathbb{R}$ by

$$F[v] := \int_{\Omega} fv \qquad \text{for } v \in \mathring{V}.$$

 V_0 is a constraint subspace with the constraint $C[i][v] := v(x_i^b) = 0$ for any boundary node x_i^b (i.e. $\mathcal{N}_H \cap \partial \Omega = \{x_1^b, ..., x_{\bar{N}}^b\}$). We can therefore identify

$$V_0 = \{ v \in V | C[i][v] = 0 \ \forall 1 \le i \le \bar{N} \} =: V_C.$$

The affine space V_{g_H} is given by

$$V_{g_H} := \left\{ v + g_H \middle| v \in V \text{ and } g_H := \sum_{i=1}^{\tilde{N}} g(x_i) \Phi_i \right\}$$

and the (differential) operator $G: V_{g_H} \to V_C'$ by

$$G(u)[v] := \int_{\Omega} \nabla u \cdot \nabla v \, dx.$$

With these notations the original problem reads:

Find
$$u \in V_{g_H}$$
 with $G(u) = F$ on V_C .

4 Programming concept

In this section we describe the general programming concept. For a detailed description of these classes, see section? and the doxygen documentation. These classes are realized in a namespace Functionals in order to avoid conflicts with other existing Dune-Fem-classes. We do not distinguish between interfaces and realizations here, this is only intended as a conceptual overview.

4.1 Functionals

Remark 4.1 (Class tree).

Functional

- ightarrow CombinedFunctional
- \rightarrow LinearFunctional
 - \rightarrow CombinedLinearFunctional
 - ightarrow CodimCFunctional
 - ightarrow IntegralFunctional

Class 4.2 (Functional).

This class represents a functional F (see definition 2.2). It provides the base class for linear and nonlinear functionals.

Class definition:

class Functional< FunctionSpaceType >

Methods:

| RangeFieldType ret = operator(FunctionType function) | | |
|--|---|--|
| description: | This method represents the functional, applied to a function. | |
| in: FunctionType function v | | |
| out: | RangeFieldType ret $F[v]$ | |

Class 4.3 (CombinedFunctional).

Given two functionals $F,G \in V'$, this class represents the functional

$$F+G:V\to\mathbb{R}$$

$$v\mapsto F[v]+G[v].$$

This class is derived from Functional.

${\it Class \ definition:}$

class CombinedFunctionalFirstFunctionalType, SecondFunctionalType >
: Functional

Methods:

| <pre>RangeFieldType ret = operator(FunctionType function)</pre> | | | |
|---|---|--|--|
| description: | This method redefines Functional::operator(). | | |
| in: | FunctionType function v | | |
| out: | RangeFieldType ret $F[v] + G[v]$ | | |

4.2 Required classes

First of all we give an overview on the various classes that are required in our concept. In particular we comment on the functionality of each class.

typedef Constraint < FunctionalType > ConstraintType;

- \circ various realizations of constraints C are possible (boundary conditions, periodicity, zero-average, ...); they are derived from the general Constraint class
- o mapping an element $v \in V$ on an element $v_C \in V_C$ is not unique, therefore 'applying a constraint' to a general function v means that we project v on V_C with respect to certain scalar product; in the discrete setting these projections are typically straight forward
- o required methods:
- · method: apply(numberOfConstraint, function) \leftrightarrow find $v_C \in V_C$ which is 'close' to v and which fulfills $C[i][v_C] = 0$, i is the index of the functional (in our functional vector), v is an analytical function
- · method: apply(numberOfConstraint, discreteFunction) \leftrightarrow find $v_C \in V_C$ which is 'close' to v_H and which fulfills $C[i][v_C] = 0$, i is the index of the functional (in our functional vector), v_H is a discrete function; typically we simply change the value of v_H in a certain number of nodes
- method: applyLocal(numberOfConstraint, localBasefunctionSet, localBasefunctionSet) → again, an abstract method depending on the specific type of the constraint; it returns local contributions for a specific grid element; it is required for assembling the system matrix in our system of equations; details are given later
- method: applyLocal(localBasefunctionSet, localBasefunctionSet)

) use applyLocal(numberOfConstraint, localBasefunctionSet, localBasefunctionSet) for all numberOfConstraint

- other methods depending on the specific type of a constraint (e.g. DirichletConstraint)?
- constraints are used to construct a 'constraint subspace' for the user, nothing else has to be done with the constraints

typedef LinearSubspace < DiscreteFunctionSpace, ConstraintType > LinearSubspaceType;

- o derived from DiscreteFunctionSpace
- all the information about the constraint is in our subspace
- we can extract the constraint that it was constructed from
- o formally the subspace is of the same size as DiscreteFunctionSpace
- in particular an object of LinearSubspace becomes the space of test functions in our later problem

typedef AffineSubspace < LinearSubspace > AffineSubspaceType;

- the space of the solution
- \circ initialized with a fixed discrete function v_H : 'AffineSubspace = v_H + LinearSubspace'
- o AffineSubspace-class derived from DiscreteFunctionSpace

typedef Operator< LinearSubspaceType, AffineSubspaceType, MatrixObjectTraits > DifferentialOperatorType;

- \circ can be derived from the dune-fem Operator-class, later it should be implemented independently
- \circ Operator : AffineSubspace \rightarrow (LinearSubspace)'
- if required: automatically assembles the correct system matrix (which is a quadratic sparse row matrix) with respect to the subspaces (i.e. with respect to the constraints)
- simplified we can say: the *linear subspace* tells us which lines we must substitute in our later system of equations and the *affine subspace* tells us by what we must substitute these lines.
- usage of a DifferentialOperatorType-object identical to the old usage of an Operator-object
- o get system matrix with operator.systemMatrix();

Algebraic classes (assembling of system matrix and right hand side):

To assemble the right hand side in our system of equations: typedef FunctionalAssembler < FunctionalType, AffineSubspace > FunctionalAssemblerType;

To assemble the correct system matrix (with respect to the subspaces): typedef OperatorAssembler < OperatorType > OperatorAssemblerType;

incorporates something like:
 assembleSystemMatrix(); constraints.apply(systemMatrix());

Both classes might be incorporated in a general FunctionalSolverInterface, so that the user does not need to care about the system assemblers.

4.3 Draft

Essential classes:

```
using namespace Functionals;
typedef Functional< DiscreteFunctionSpace > FunctionalType;
typedef Constraint < FunctionalType > ConstraintType;
typedef LinearSubspace < DiscreteFunctionSpace, ConstraintType > LinearSubspaceType;
typedef AffineSubspace < LinearSubspace > AffineSubspaceType;
// sparse row matrix of size N \times N
typedef Dune::SparseRowMatrixTraits < DiscreteFunctionSpace, DiscreteFunctionSpace
> MatrixObjectTraits;
typedef Operator< LinearSubspaceType, AffineSubspaceType,</pre>
   MatrixObjectTraits > DiffOperatorType;
// algebraic system assemblers:
typedef OperatorAssembler < OperatorType > OperatorAssemblerType;
typedef FunctionalAssembler < FunctionalType, AffineSubspace > FunctionalAssemblerType;
// CG scheme
typedef CGInverseOp< DiscreteFunctionType, OperatorAssembler > InverseOperatorType;
Main code:
DiscreteFunctionType rhs( "right hand side", discreteFunctionSpace );
// use a right hand side assembler class to apply 'functional+constraints' to right hand
side vector
FunctionalAssemblerType rhsAssembler ( functional, affineSubspace );
```

```
rhsAssembler.assemble( rhs );
// behaves like the old Operator-class of Dune-Fem:
OperatorAssemblerType systemMatrixAssembler ( differentialOperator );
// 'differentialOperator' contains correct 'systemMatrix()':
InverseOperatorType cg( systemMatrixAssembler, 1e-6, 1e-8 );
cg( rhs, solution );
We might think about hiding this main code behind a 'FunctionalSolver-
Interface', so that the user can simply call:
   cg( differentialOperator, functional, affineSubspace, solution );
(i.e. FunctionalSolverInterface < Operator, Functional, AffineSubspace >
Comparison with 'old' main code (for laplace operator and zero boundary
condition):
DiscreteFunctionType rhs( "rhs", discreteFunctionSpace );
AssembledFunctional < Functional Type > rhsFunctional ( disceretFunctionSpace, functional
rhsFunctional.assemble( rhs );
typedef LaplaceOperator < DiscreteFunctionType, MatrixObjectTraits > LaplaceOperatorType;
// apply constraints
bool hasDirBoundary = constraints.apply( laplaceOperator.systemMatrix(), rhs,
solution );
InverseOperatorType cg( laplaceOperator, 1e-6, 1e-8 );
cg( rhs, solution );
```

The essential difference is that the (differential) operator already knows the correct system matrix (due to the subspaces, that know the constraints). Therefore the user does not need some kind of 'constraints.apply' method (this happens internally in the two system assemblers).

5 Realization of Functionals

Class 5.1 (Functional < Space >).

Represents a functional f. This class comes without any functionality at the moment, until someone comes up with a reasonable example of nonlinear functionals.

```
number = operator( function ) | Given u, returns f[u].
```

5.1 Linear Functionals

Definition 5.2 (Linear functional).

Let V be a vector space, \mathbb{K} its underlying scalar field and f a functional. If, for all $u,v \in V$ and for all $\lambda,\mu \in \mathbb{K}$,

$$f[\lambda u] + f[\mu v] = \lambda f[u] + \mu f[v] \tag{5.1}$$

holds, f is called a linear functional.

Definition 5.3 (Dual Space).

Let V be a vector space and \mathbb{K} its underlying scalar field. The space

$$V^* := \{ f : V \to \mathbb{K} | f \ linear functional \}$$

is called the dual space of V and is a vector space itself.

Lemma 5.4 (Localization property of linear functionals).

Let V_G be a discrete function space ([1, Def. 18]) and $f \in V_G^*$ a linear functional. Let further be

$$u = \sum_{E \in G} \sum_{i \in I_E} u_i^E \varphi_i^E \tag{5.2}$$

the representation for a $u \in V_G$ in terms of its local DoFs u_i^E and the local base functions φ_i^E ([1, Def. 20]). Then it holds that

$$f[u] = \sum_{E \in G} \sum_{i \in I_E} u_i^E f\left[\varphi_i^E\right],\tag{5.3}$$

which can also be written as

$$f[u] = \sum_{E \in G} u^E \cdot f[B_E]^E, \tag{5.4}$$

where $u^E := (u_i^E)_{i \in I_E}$ is the local DoF vector of u on E and $f[B_E]^E$ is defined as the vector

$$f[B_E]^E := \left(f \left[\varphi_i^E \right] \right)_{i \in I_E} \tag{5.5}$$

for a local basfunction set B_E .

Class 5.5 (LinearFunctional < Space, DiscreteFunctionSpace >:Functional).

Represents a linear functional f.

| number | Redefines Functional::operator(). |
|--------------------------------------|--|
| = operator(function) | Given u , computes $\sum u^{\bar{E}} \cdot f[B_E]^E$ |
| - | $E \in G$ |
| | by doing a gridwalk and calling |
| | applyLocal() on each entity. |
| vector | Implements $f[B_E]^E$. |
| = applyLocal(localBasefunctionSet) | Given B_E , computes $(f[\varphi_i^E])_{i \in I_E}$ |

5.2 Integral Functionals

Definition 5.6 (Integral functional).

Let V be a vector space, $u \in V$ and $f \in V^*$. If f[u] can be decomposed as

$$f[u] = \sum_{c=0}^{\dim} f^c[u], \tag{5.6}$$

where $f^c \in V^*$ are codim c integral functionals, which can be written as

$$f^{c}[u] = \int_{-\infty} \tilde{f}^{c}[u] \tag{5.7}$$

for a set ω^c of codimension c and a functional $\tilde{f}^c \in V^*$, then f is called an integral functional.

Lemma 5.7 (Localization property of integral functionals).

Let V_G be a discrete function space and $f \in V_G^*$ an integral functional. Then it holds that

$$f[u] = \sum_{E \in G^0} \sum_{i \in I_E} u_i^E \sum_{c=0}^{dim} f^c[\varphi_i^E]$$
$$= \sum_{E \in G^0} u^E \cdot \left(\sum_{c=0}^{dim} \int_{G_c^0} \tilde{f}^c[B_E]^E\right), \tag{5.8}$$

where (...) is to be understood as the vector

$$\left(\sum_{c=0}^{\dim} \int_{G_E^0} \tilde{f}^c[B_E]^E\right) := \left(\sum_{c=0}^{\dim} \int_{G_E^c} \tilde{f}^c[\varphi_i^E]\right)_{i \in I_E},\tag{5.9}$$

where G_E^c is "the set of all codim c entities, that lie inside E".

Class 5.8 (LocalOperationProvider).

Represents the operation $\tilde{f}^c[\varphi_i^E]$, e.g. $\tilde{f}^c[\varphi_i^E] = f(x)\varphi_i^E(x)$. This class has to be provided by the user in order to define a CodimIntegralFunctional (see below).

| number | Given a point x in local coordinates, returns $\tilde{f}^c[\varphi_i^E](x)$, |
|-------------------------------------|---|
| = apply(function, | where φ_i^E is given as function and some function |
| localPoint, | associated with the functional can be given as |
| <pre>functionalFunction = 1)</pre> | functionalFunction |

Class 5.9 (CodimIntegralFunctional < LocalOperationProvider >: LinearFunctional). Represents a codim c functional $f^c[u]$. A CodimIntegralFunctional provides an additional method prepareLocalIntegration() to facilitate the integration in

IntegralFunctional::applyLocal() (see below). There should be derived classes for each codimension, which, together with a suitable LocalOperationProvider, can be given to an IntegralFunctional to provide something like an L2Functional for the user.

| number | Inherited from LinearFunctional. |
|--------------------------------------|---|
| = operator(function) | |
| vector | Redefines LinearFunctional::applyLocal(). |
| = applyLocal(localBasefunctionSet) | Given B_E , computes $(f^c[\varphi_i^E])_{i \in I_E}$ by |
| | doing a codim c integration by quadrature |
| | $and \ calling \ {\tt prepareLocalIntegration}$ |
| | for each quadrature point. |
| vector | Given B_E and a point x in local |
| = prepareLocalIntegration(| coordinates, returns $\tilde{f}^c[\varphi_i^E](x)$ by calling |
| localBasefunctionSet | $the \ underlying \ {	t Local Operation Provider}.$ |
| localPoint) | |

Class 5.10 (IntegralFunctional < CodimIntegralFunctionals >: LinearFunctional). Represents an integral functional. This is like a CombinedLinearFunctional (see somewhere), but the integration in applyLocal() is only done once, calling

prepareLocalIntegration() on each CodimIntegralFunctional.

| number | Inherited from LinearFunctional. |
|--------------------------------------|--|
| = operator(function) | |
| vector | Redefinition of |
| = applyLocal(localBasefunctionSet) | LinearFunctional::applyLocal(). |
| | Given B_E , computes $(f^c[\varphi_i^E])_{i \in I_E}$ by |
| | doing a codim c integration for each given |
| | codim by quadrature and calling |
| | prepareLocalIntegration() of each |
| | CodimIntegralFunctional for each |
| | quadrature point. |

6 Realization of Constraints

Maybe, we should discuss the general concept first.

 $\label{thm:example:constraint} Example: \texttt{ConstraintType::DirichletConstraint dirConstraint(function)};$

References

[1] A. Dedner, R. Klöfkorn, M. Nolte, and M. Ohlberger. A generic interface for parallel and adaptive discretization schemes: abstraction principles and the dune-fem module. *Computing*, 90(3-4):165–196, 2010.