# 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/`.

## Contents

## 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*

$$
\begin{aligned}
-\nabla \cdot \left( a\nabla u \right) &= f && \text{in } \Omega, & (1.1) \\
u &= g && \text{on } \partial\Omega.
\end{aligned}
$$

**Definition 1.2.** *Weak formulation*
*Let $H^1$ and $H_0^1$ be given as usual and let $H_g^1$ for $g \in H^1$ be defined as*

$$
H_g^1 := \left\{ v \in H^1 \,\middle|\, v = w + g \text{ for a } w \in H_0^1 \right\}.
$$

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

$$
\int_\Omega a\nabla u \nabla v \, dx = \int_\Omega fv \, dx \qquad \text{for all } v \in H_0^1. \qquad (1.2)
$$

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*

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

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

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

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

$$
\begin{aligned}
A(u) : H_0^1 &\to \mathbb{R} \\
v &\mapsto A(u)[v] := \int_\Omega a\nabla u \nabla v \, dx.
\end{aligned}
$$

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 follows. Find $u \in H_g^1$, such that*

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

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 Abstract concept

## 2.1 Functionals

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*

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

*is called a* functionspace*. If $V$ is an $\mathbb{R}$–vector space, $V$ is called a* linear functionspace*.*

**Definition 2.2** (Functional)**.**
 *Let $V$ be a function space. A map*

$$F : V \to \mathbb{R},$$
$$v \mapsto F[v] \qquad (2.1)$$

*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*

$$V' := \left\{ F : V \to \mathbb{R} \big| F \textit{ is a linear functional } \right\} \qquad (2.2)$$

*is called the dual space of $V$.*

**Lemma 2.3** (Localization property of discrete linear functionals)**.**

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

$$u = \sum_{E \in G} u_E \tag{2.3}$$

the representation for a $u \in V_G$ in terms of its local functions $u_E := u_{|E}$ and

$$u_E = \sum_{i \in I_E} u_i^E \varphi_i^E \tag{2.4}$$

the representation of a local function in terms of its local DoFs $u_i^E$ and the local base functions $\varphi_i^E$ ([1, Def. 20]). Thus, $u_E$ can be written as

$$u = \sum_{E \in G} \sum_{i \in I_E} u_{\mu_G(i)}^E \varphi_{\mu_G(i)}^E,$$

where $\mu_G$ is local–to–global DoF mapping ([1, Def. 18]). Since $F$ is a discrete linear functional, it holds that

$$F[u] = \sum_{E \in G} \sum_{i \in I_E} u_{\mu_G(i)}^E F\Big[\varphi_{\mu_G(i)}^E\Big], \tag{2.5}$$

which can also be written as

$$F[u] = \sum_{E \in G} u^E \cdot F[B_E]^E, \tag{2.6}$$

where $u^E := (u_{\mu_G(i)}^E)_{i \in I_E}$ is the local DoF vector of $u_E$ (mapped to global) and $F[B_E]^E$ is defined as the vector

$$F[B_E]^E := \left( F\Big[\varphi_{\mu_G(i)}^E\Big] \right)_{i \in I_E} \tag{2.7}$$

for a local basefunction set $B_E$.

An important set of linear functionals is the set of those functionals that are associated with integration, e.g the functional $F$, induced by the function $f$, which arises as a right hand side in the introductory example (see definition 1.3). To formulate the abstract idea of an "integral functional", we first have to introduce a "codim $c$ functional", which is associated with integration over a set of codimension $c$.

**Definition 2.4** (Codim $c$ functional)**.**
*Let $V_G$ be a discrete function space and $F \in V'_G$ a discrete linear functional.
If $F[v]$ can be written as*

$$F[v] = \int\limits_{\omega^c} \tilde{f}[v](x) \ dx$$

*for a function $v \in V_G$, a subset $\omega^c \subset \Omega$ of codimension $c$ and a map*

$$\tilde{f} : V_G \to V_G,$$

*$F$ is called a* codim $c$ functional*. The map $\tilde{f}$ is called a* local operation
provider*.*

Given suitable codim $c$ functionals for all codimensions of interest we
can now define an integral functional as a combination of those codim $c$
functionals.

**Definition 2.5** (Integral functional)**.**
*Let $V_G$ be a discrete function space, $F^{c_1}, \ldots, F^{c_C} \in V'_G$ codim functionals for
the codimensions $c_1, \ldots, c_C \in \mathbb{N}^{\geq 0}$ and $F \in V'_G$ a discrete linear functional.
If $F[v]$ can be written as*

$$F[v] = \sum_{c=c_1}^{c_C} F^c[v]$$

*for a function $v \in V_G$, $F$ is called an* integral functional*.*

**Remark 2.6** (Localization property of integral and codim $c$ functionals)**.**
*Since integral functionals and codim $c$ functionals are themselves discrete
linear functionals we can localize the evaluation of these functionals as in
lemma 2.3.*

## 2.2  Constraints and subspaces

**Definition 2.7** (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*

$$C : \{1, ..., M\} \times V \to \mathbb{R} \ \ with \ (i,v) \mapsto C[i][v] := F_i[v]. \tag{2.8}$$

*The condition:*

$$C[i][v] = 0 \ \ \forall 1 \leq i \leq M \tag{2.9}$$

*is called a* Constraint *for $v$.*

In particular each linear functional implies a constraint.

**Definition 2.8** (Linear subspace).
*Let $V$ be a linear function space and $C[\cdot][\cdot] = 0$ a constraint on $V$. Then we call*

$$V_C := \{v \in V \mid C[i][v] = 0 \ \forall i \in \{1, ..., M\}\} \tag{2.10}$$

*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 2.9** (Affine subspace).
*Let $V$ be a function space, $V_C$ a linear subspace and $g \in V$. Then we call*

$$V_g := \{v + g \mid v \in V_C\} \subset V \tag{2.11}$$

*an* affine subspace *with respect to $g$ and $V_C$.*

In general, $V_g$ is only a subspace of $V$ and not a linear subspace (in the sense, that $V_G$ is not a vector space itself in general ). It will be the space of solutions in our later problem.

## 2.3 Operators

**Definition 2.10** (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 subspace. Then we call*

$$G : V_g \to V'_C \tag{2.12}$$

*an* operator *on $V_g$. If*

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

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

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

**Problem 2.11** (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 subspace. Find $u \in V_g$, such that*

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

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*

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

*(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

$$F[v] := \int_\Omega fv \qquad \text{for } v \in V_0.$$

$V_0$ 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 subspace $V_{g_H}$ 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:

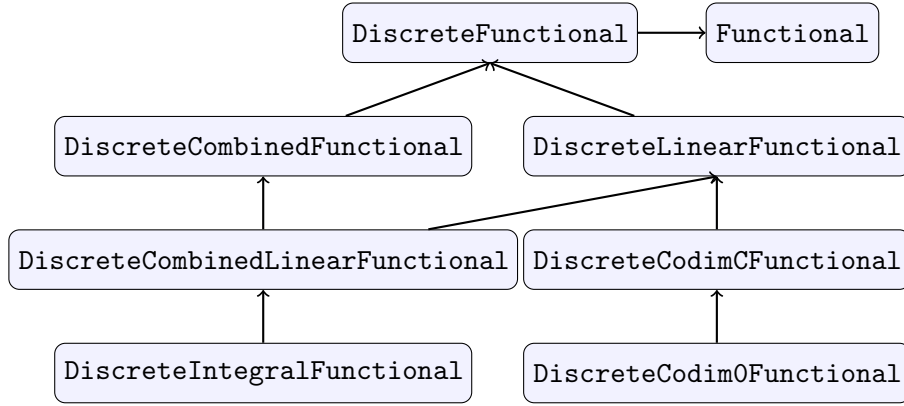$$\text{Find } u \in V_{g_H} \text{ with } G(u) = F \text{ on } V_C.$$

# 4 Realization in Dune-Fem-Functionals

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

The following diagram is intended to be a conceptual overview only. It is not intended to display a class hierarchy.

**Remark 4.1** (Conceptual class tree).

```
                    ┌─────────────────────┐      ┌──────────────┐
                    │ DiscreteFunctional  │─────▶│  Functional  │
                    └─────────────────────┘      └──────────────┘
                              ▲
            ┌─────────────────┴──────────────┐
┌───────────────────────────┐    ┌───────────────────────────┐
│ DiscreteCombinedFunctional│    │  DiscreteLinearFunctional │
└───────────────────────────┘    └───────────────────────────┘
            ▲                              ▲
            │               ┌──────────────┤
┌───────────────────────────────┐  ┌───────────────────────────┐
│ DiscreteCombinedLinearFunctional│  │  DiscreteCodimCFunctional │
└───────────────────────────────┘  └───────────────────────────┘
            ▲                              ▲
┌───────────────────────────┐    ┌───────────────────────────┐
│ DiscreteIntegralFunctional│    │  DiscreteCodim0Functional │
└───────────────────────────┘    └───────────────────────────┘
```

The class `Functional` will not really be used. It is only there to provide us with the possibility to have all the following classes in a non–discrete way in the future. The only thing this class does is to enforce the `operator()` for all functionals. The only method, the function $v$ has to provide, is a method `evaluate( xGlobal )`.

**Class 4.2** (`Functional`).
*This class represents a functional $F$ (see definition 2.2). It provides the base class for discrete and what–ever–else–there–will–be functionals.*

### *Class definition:*

```
class Functional< FunctionSpaceType >
```

### *Methods:*

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

The class `DiscreteFunctional` is the actual base class for all functionals we use at the time being.

**Class 4.3** (`DiscreteFunctional`).
*This class represents a functional F (see definition 2.2), which can be applied to a discrete function.*

### *Class definition:*

```
class DiscreteFunctional< DiscreteFunctionSpaceType >
```

### *Methods:*

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

The `DiscreteCombinedFunctional` is more or less a pair of two `DiscreteFunctional`s. When its `operator()` is called, it just calls each `operator()` and adds the results.

**Class 4.4** (`DiscreteCombinedFunctional`).
*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* `DiscreteFunctional`.

### *Class definition:*

```
class DiscreteCombinedFunctional<
 FirstFunctionalType,
 SecondFunctionalType >
 :  Functional
```

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| RangeFieldType ret = operator(<br>DiscreteFunctionType discreteFunction ) | | |
|---|---|---|
| *description:* | *This method redefines* `DiscreteFunctional::`<u>`operator`</u>`().` | |
| *in:* | `DiscreteFunctionType discreteFunction` | $v$ |
| *out:* | `RangeFieldType ret` | $F[v] + G[v]$ |

The `DiscreteLinearFunctional` is the base class for a wide range of interesting functionals – linear functionals. As stated in lemma 2.3, the most important property of linear functionals is, that its application to a discrete function can be split up and carried out by some kind of local application of the functionals to a local function.

**Class 4.5** (`DiscreteLinearFunctional`).
*This class represents a linear functional F (see definition 2.2). All linear functionals have to provide the method* `applyLocal()` *in addition to the method* `operator()`. *This class is derived from* `DiscreteFunctional`.

*Class definition:*

```
class DiscreteLinearFunctional< DiscreteFunctionSpaceType >
: DiscreteFunctional
```

*Methods:*

| RangeFieldType ret = operator(<br>DiscreteFunctionType discreteFunction ) | | |
|---|---|---|
| *description:* | *This method redefines* `DiscreteFunctional::`<u>`operator`</u>`().` *It makes use of the localization property of linear functionals (see lemma 2.3). It is implemented as a grid walk over all codim 0 entities which calls the method* `applyLocal()` *on each entity. Thus each linear functional only has to implement the method* `applyLocal()`. | |
| *in:* | `DiscreteFunctionType discreteFunction` | $v$ |
| *out:* | `RangeFieldType ret` | $F[v]$ |

```
void applyLocal(
 LocalBasefunctionSetType localBasefunctionSet,
 LocalDoFVectorType returnVector )
```

| | |
|---|---|
| *description:* | *Given the localization property of a linear functional (see lemma 2.3), this method implements the vector $F[B_E]^E$. This is still only a rough idea of this methods signature. It is highly possible that we will need to extend this method to take additional arguments, such as the neighbors local basefunction set etc...* |
| *in:* | `LocalBasefunctionSetType localBasefunctionSet`<br>$B_E$ |
| *out:* | `LocalDoFVectorType returnVector`<br>$F[B_E]^E := \left( F\left[ \varphi^E_{\mu_G(i)} \right] \right)_{i \in I_E}$ |

## 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;`

- ○ various realizations of constraints $C$ are possible (boundary conditions, periodicity, zero-average, ...); they are derived from the general `Constraint` class

- ○ 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

- ○ required methods:

- · 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 )` $\rightarrow$ 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 )` $\rightarrow$ use `applyLocal( numberOfConstraint, localBasefunctionSet, localBasefunctionSet )` for all `numberOfConstraint`

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- 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;
```

- derived from `DiscreteFunctionSpace`

- all the information about the constraint is in our subspace

- we can extract the constraint that it was constructed from

- 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, DiscreteFunctionType >
AffineSubspaceType;
```

- the space of the solution

- initialized with a fixed discrete function $v_H$: 'AffineSubspace $= v_H +$ LinearSubspace'

- `AffineSubspace`-class derived from `DiscreteFunctionSpace`

```
typedef Operator< LinearSubspaceType, AffineSubspaceType, MatrixObjectTraits
> DifferentialOperatorType;
```

- can be derived from the dune-fem Operator-class, later it should be implemented independently

- 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

- *Algebraic representation:* get system matrix with `operator.systemMatrix();` or `operator.algebraic();`

- ○ incorporates something like:
  `SystemMatrix(); constraints.apply( systemMatrix() );`, `algebraic();`
  `constraints.apply( algebraic() );` respectively

`typedef FunctionalAssembler< FunctionalType, AffineSubspace >`
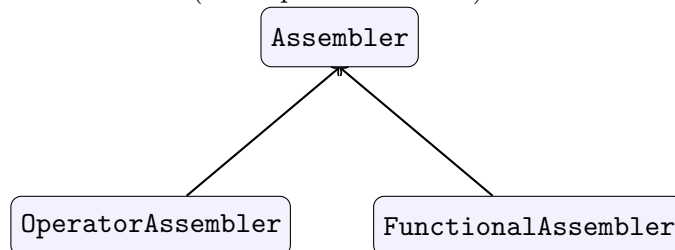`FunctionalAssemblerType;`

- ○ assembles the right hand side in our system of equations

- ○ *Algebraic representation:* get assembled functional with `functional.algebraic()`

- ○ incorporates something like:
  `algebraicl(); constraints.apply( functional );`

Both classes (`DifferentialOperator` and `FunctionalAssembler`) might
be incorporated in a general `FunctionalSolverInterface`, so that the user
does not need to care about the system assemblers.

### 4.2.1 Suggestion for an alternative "Assembler" design

Maybe we should think about the operator and "assembled functional" design again. Here is another abstract approach:

**Remark 4.6** (Conceptual class tree)**.**



`typedef Assembler < AssemblerTraits > AssemblerType;`

- ○ Assembler interface class.

- ○ Each class derived from this interface defines a type `AlgebraicRepresentationType`,
  which defines how the algebraic representation is stored - for example
  a vector or matrix.

- ○ A method `algebraic()` with return type `AlgebraicRepresentationType`
  is introduced here.

`typedef OperatorAssembler< LinearSubspaceType, AffineSubspaceType>`
`OperatorAssemblerType;`

- ○ Derived from `Assembler`.

- $\circ$ typedef MatrixObject AlgebraicRepresentationType.

- $\circ$ The method `algebraic()` represents the algebraic representation for the system matrix, i.e. the assembled system matrix.

```
typedef FunctionalAssembler < FunctionalType, AffineSubspace >
FunctionalAssemblerType;
```

- $\circ$ Derived from `Assembler`.

- $\circ$ typedef VectorObject AlgebraicRepresentationType.

- $\circ$ The method `algebraic()` represents the algebraic representation, i.e. the assembled functional.

No we can define the `Operator` and `FunctionalAssembler` in a different way:
```
typedef Operator< FunctionalType, AffineSubspace, AssemblerType
> DifferentialOperatorType;
```
Note: We can also define `typedef Operator< AssemblerType > DifferentialOperatorType` by extracting the space types from the assembler.

- $\circ$ Same properties as above...

- $\circ$ Define a private method `void applyConstraints(algebraicRepresentation)` where the constraints are extracted and applied to the algebraic representation. Now we can implement a general assemble method just by writing `applyConstraints(operator.algebraic())`.

```
typedef RHSFunctional< FunctionalType, AffineSubspace, AssemblerType
>
RHSFunctionalType;
```
Note: We can also define `typedef RHSAssembler< AssemblerType > RHSAssemblerType` by extracting the space types from the assembler.

- $\circ$ Same properties as above...

- $\circ$ Define a private method `applyConstraints(algebraicRepresentation)` where the constraints are extracted and applied to the algebraic representation. Now we can implement a general assemble method just by writing `applyConstraints(functional.algebraic())`.

## 4.3 Draft

```
1  using namespace Functionals;
2
3  typedef Functional < DiscreteFunctionSpace > FunctionalType;
4  typedef Constraint < FunctionalType > ConstraintType;
5  typedef LinearSubspace < DiscreteFunctionSpace , ConstraintType >
```

```
6      LinearSubspaceType ;
7  typedef AffineSubspace < LinearSubspace > AffineSubspaceType ;
8
9  // sparse row matrix of size N x N
10 typedef Dune :: SparseRowMatrixTraits < DiscreteFunctionSpace , DiscreteFunctionSpace >
11    MatrixObjectTraits ;
12 typedef Operator < LinearSubspaceType , AffineSubspaceType , MatrixObjectTraits >
13    DiffOperatorType ;
14
15 // algebraic system assembler :
16 typedef FunctionalAssembler < FunctionalType , AffineSubspace >
17    FunctionalAssemblerType ;
18
19 MatrixObjectTraits > DiffOperatorType ;
20 // CG scheme
21 typedef CGInverseOp < DiscreteFunctionType , OperatorAssembler >
22    InverseOperatorType ;
```

Main Code:

```
1  // constraints , for example dirichlet constraints
2  ConstraintsType constraints ( gridPart );
3
4  // subspaces
5  LinearSubspaceType linearSubspace ( constraints );
6  AffineSubspaceType affineSubspace ( linearSubspace , discretefunction );
7
8  // operator (behaves like the old Operator - class of dunefem)
9  DiffOperatorType differentialOperator ( linearSubspace , affineSubspace );
10
11 DiscreteFunctionType rhs ( "right hand side", discreteFunctionSpace );
12
13 // use a right hand side assembler class to apply 'functional+constraints '
14 // to right hand side vector
15 FunctionalAssemblerType rhsAssembler ( functional , affineSubspace );
16 rhsAssembler . algebraic ( rhs );
17
18 // 'differentialOperator ' contains correct 'systemMatrix ()':}
19 InverseOperatorType cg ( differentialOperator , 1e -6, 1e -8 );
20 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 to the old main code (for laplace operator and zero boundary condition):

```
1  DiscreteFunctionType rhs ( "rhs", discreteFunctionSpace );
2  typedef AssembledFunctional < FunctionalType > AssembledFunctionalType ;
3  AssembledFunctionalType rhsFunctional ( discretFunctionSpace , functional );
4  rhsFunctional . assemble ( rhs );
5
```

```
6   typedef LaplaceOperator< DiscreteFunctionType , MatrixObjectTraits >
7     LaplaceOperatorType ;
8
9   // apply constraints
10  bool hasDirBoundary =
11    constraints.apply( laplaceOperator.systemMatrix(), rhs, solution );
12
13  InverseOperatorType cg( laplaceOperator , 1e-6, 1e-8 );
14  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

## 5.1 Integral Functionals

**Definition 5.1** (Integral functional).
*Let $V$ be a vector space, $u \in V$ and $f \in V^*$. If $f[u]$ can be decomposed as*

$$f[u] = \sum_{c=0}^{dim} f^c[u], \qquad (5.1)$$

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

$$f^c[u] = \int_{\omega^c} \tilde{f}^c[u] \qquad (5.2)$$

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

**Lemma 5.2** (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*

$$f[u] = \sum_{E \in G^0} \sum_{i \in I_E} u_i^E \sum_{c=0}^{dim} f^c[\varphi_i^E]$$

$$= \sum_{E \in G^0} u^E \cdot \left( \sum_{c=0}^{dim} \int_{G_E^0} \tilde{f}^c[B_E]^E \right), \qquad (5.3)$$

*where $(\dots)$ is to be understood as the vector*

$$\left( \sum_{c=0}^{dim} \int_{G_E^c} \tilde{f}^c[B_E]^E \right) := \left( \sum_{c=0}^{dim} \int_{G_E^c} \tilde{f}^c[\varphi_i^E] \right)_{i \in I_E}, \qquad (5.4)$$

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

**Class 5.3** (`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`<br>`= apply( function,`<br>`localPoint,`<br>`functionalFunction = 1 )` | *Given a point x in local coordinates, returns $\tilde{f}^c[\varphi_i^E](x)$,
where $\varphi_i^E$ is given as `function` and some function
associated with the functional can be given as
`functionalFunction`* |

**Class 5.4** (`CodimIntegralFunctional< LocalOperationProvider >:LinearFunctional`).
*Represents a codim c functional $f^c[u]$. A `CodimIntegralFunctional` pro-
vides 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`<br>`= operator( function )` | *Inherited from `LinearFunctional`.* |
| `vector`<br>`= applyLocal( localBasefunctionSet )` | *Redefines `LinearFunctional::applyLocal()`.
Given $B_E$, computes $(f^c[\varphi_i^E])_{i \in I_E}$ by
doing a codim c integration by quadrature
and calling `prepareLocalIntegration()`
for each quadrature point.* |
| `vector`<br>`= prepareLocalIntegration(`<br>`localBasefunctionSet`<br>`localPoint )` | *Given $B_E$ and a point x in local
coordiantes, returns $\tilde{f}^c[\varphi_i^E](x)$ by calling
the underlying `LocalOperationProvider`.* |

**Class 5.5** (`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`.*

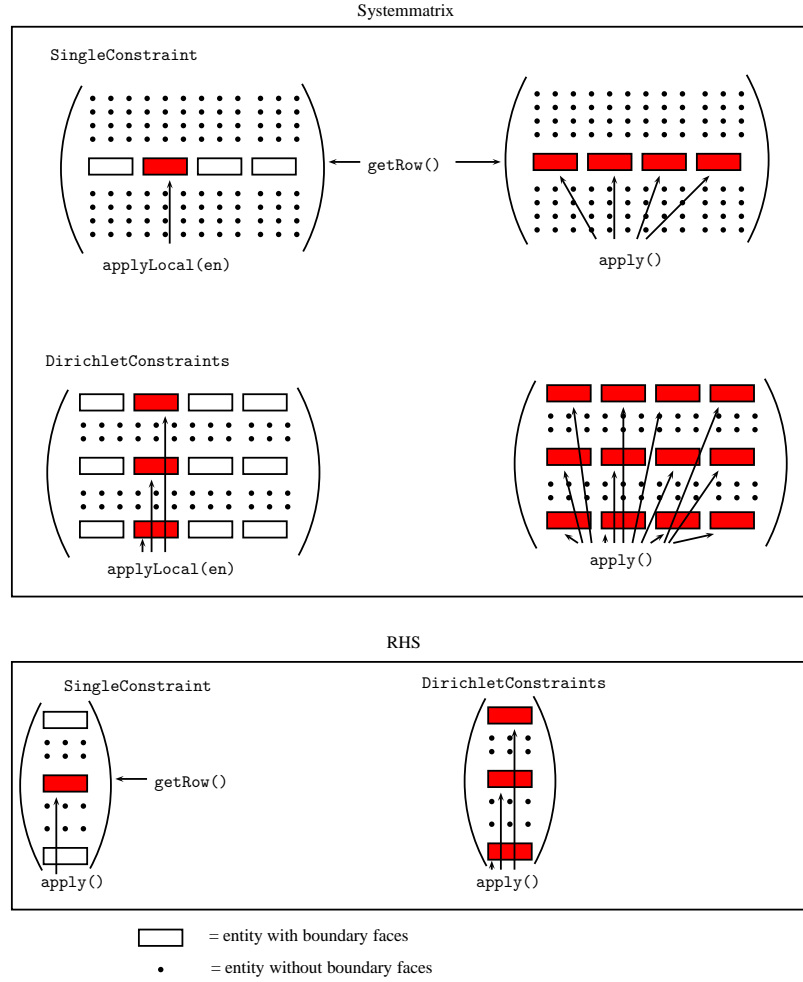| | |
|---|---|
| `number`<br>`  = operator( function )` | *Inherited from* `LinearFunctional`. |
| `vector`<br>`  = applyLocal( localBasefunctionSet )` | *Redefinition of* `LinearFunctional::applyLocal()`. *Given* $B_E$, *computes* $(f^c[\varphi_i^E])_{i \in I_E}$ *by doing a codim c integration for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

# 6 Realization of Constraints

We should discuss about the general concept, especially about the methods `operator()`, `apply()` and `applyLocal()`.

**Remark 6.1** (Conceptual class tree)**.**
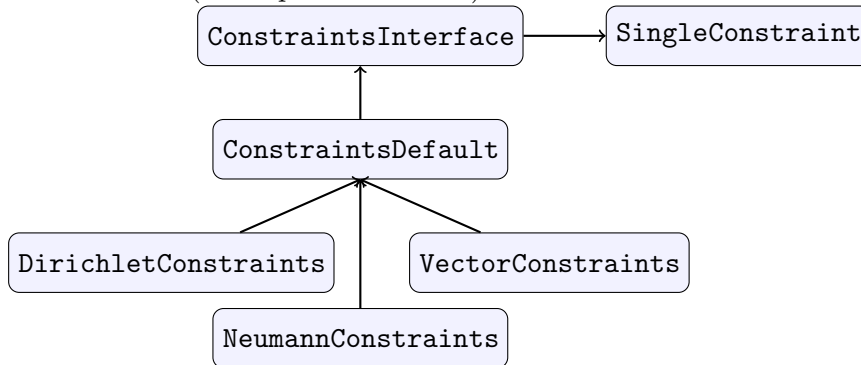


**Remark 6.2** (SingleConstraint vs. ConstraintsInterface)**.**
*The next figure shows the class concept again - concentrating on the difference between a single constraint and classes derived from the class* `ConstraintsInterface`. *Here we should discuss about some implementation details, especially about the Interface class. (Is it convient to implement a method like* `applyLocal(en)`*?)*

Systemmatrix

SingleConstraint

getRow()

applyLocal(en)

apply()

DirichletConstraints

applyLocal(en)

apply()

RHS

SingleConstraint

DirichletConstraints

getRow()

apply()

apply()

☐ = entity with boundary faces

• = entity without boundary faces

**Class 6.3** (`SingleConstraint< FunctionalImp >`). *Represents a single constraint. Mainly, this class is the formal implementation of 2.7. This class is the basic class for all other classes dealing with constraints. Normally this class is not used directly because an efficient implementation is not possible.*
*Shortly said, a single constraint presents a pair of a* functional *(defining the constraint) and* row number *determing the row which has to be deleted in the system matrix.*
*This means, that a class (for example representing the dirichlet constraints) can be (formally) seen as a vector of* `SingleConstraints`.

19

| | |
|---|---|
| number<br> = operator( discretefunction ) | *Computes $F[v]$, where $F$ is the functional and $v$ the discrete function.* |
| vector<br> = apply( discreteFunction) | *just calls* applyLocal() *for each entity.* |
| localVector<br> = applyLocal( entity,<br> localBasefunctionSet ) | |
| int<br> = getRow() | *returns the row number which has to be deleted in the system matrix.* |
| functional<br><br> = getFunctional() | *returns the functional representing the constraint, i.e. $F[v] \overset{!}{=} 0$ for the functional $F$ returned by this function.* |

**Class 6.4** (ConstraintsInterface< FunctionalImp >). *This class represents an interface for all classes. Mention that it is possible to write something like this:* ConstraintsInterfaceImp C; C[i].apply();.

| | |
|---|---|
| number<br> = operator( discretefunction ) | *Computes $F[v]$, where $F$ is the functional and $v$ the discrete function.* |
| vector<br> = apply( discreteFunction) | *just calls* applyLocal() *for each entity.* |
| localVector<br> = applyLocal( entity,<br> localBasefunctionSet ) | |
| int<br> = size() | *Returns number of constraints.* |
| singleconstraint<br> = operator[i] | *Returns a single constraint represented by the class* SingleConstraint. *This method will not be used in general.* |

**Class 6.5** (ConstraintsDefault< FunctionalImp >). *Default implementation of* ConstraintsInterface.

**Class 6.6** (DirichletConstraints< FunctionalImp >). *An example for constraints: Implementation of Dirichlet constraints.*
*Derived from* ConstraintsDefault. *Here we will* overwrite *the methods* operator(), apply() *and* applyLocal() *without using the single constraints from* SingleConstraint.

| | |
|---|---|
| `number`<br>`  = operator( discretefunction )` | *Computes $F[v]$, where $F$ is the functional and $v$ the discrete function.* |
| `vector`<br>`  = apply( discreteFunction)` | *just calls* `applyLocal()` *for each entity.* |
| `localVector`<br>`  = applyLocal( entity,`<br>`  localBasefunctionSet )` | |
| `int`<br>`  = size()` | *Returns number of constraints.* |
| `singleconstraint`<br>`  = operator[i]` | *Returns a single constraint represented by the class* `SingleConstraint`. *This method will not be used in general.* |

**Class 6.7** (`NeumannConstraints< FunctionalImp >`). *An example for constraints: Implementation of Neumann constraints.*
*Derived from* `ConstraintsDefault`. *See above.*

**Class 6.8** (`VectorConstraints< FunctionalImp >`). *An example for constraints: Here the constraints are stored explicitly in a vector of elements from the class* `SingleConstraint`. *Derived from* `ConstraintsDefault`. *In general we do not want to have such a class.*

# 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.