Journées 2023 du GT SCALP ($\in$ GDR IM)
Orléans

Formalization of Applied Mathematics: a journey

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My journey

In my journey, I was lucky to travel with

- François Clément,
- Florian Faissole,
- Vincent Martin,
- Micaela Mayero,
- Houda Mouhcine.

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In my other life,
I have been busy with computer arithmetic and *agrégation d'informatique*.
Do not hesitate to reach me for one of these topics.

Outline

Introduction

Mathematics

$\mathbb{R}$, $\int$, $\frac{\partial^2 u}{\partial t^2}$
theorems

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$\mathfrak{Mathematics}$	$\mathbb{R}$, $\int$, $\frac{\partial^2 u}{\partial t^2}$ theorems
Applied Mathematics	numerical scheme, convergence algorithms + theorems

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Applied Mathematics	numerical scheme, convergence algorithms + theorems
Computer	floating-point numbers, implementation programs + ?

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Computer

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Motivations

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$\Rightarrow$ nuclear simulation
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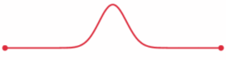
⇒ real program implementing the scheme/method

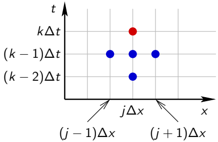
Let us machine-check this kind of programs!

1D wave equation resolution by the 3-point scheme

$$\frac{\partial^2 u(x,t)}{\partial t^2} - c^2 \frac{\partial^2 u(x,t)}{\partial x^2} = s(x,t)$$

$$\frac{u_j^k - 2u_j^{k-1} + u_j^{k-2}}{\Delta t^2} - c^2 \frac{u_{j+1}^{k-1} - 2u_j^{k-1} + u_{j-1}^{k-1}}{\Delta x^2} = s_j^{k-1}$$






```
du = u[i+1][k] - 2 * u[i][ k]  + u[i-1][k];
u[i][ k+1] = 2 * u[i][k]  - u[i][k-1] + a * du;
```

Rounding error: $\left|u_i^k - exact\left(u_i^k\right)\right| \leqslant 78 \times 2^{-53} \times (k+1) \times (k+2)$

Method error: $\left\|e_h^{k_{\Delta t}(t)}\right\|_{\Delta x} = O_{\substack{t \in [0, t_{\max}], (\Delta x, \Delta t) \to 0 \\ 0 < \Delta x \,\wedge\, 0 < \Delta t \,\wedge\, c\frac{\Delta t}{\Delta x} \leqslant 1 - \xi}} (\Delta x^2 + \Delta t^2)$

Program error: no illicit memory access, no division by zero, no overflow...

Formal verification of 32 lines of C code + 154 lines of annotations
$\hookrightarrow$ 150 theorems to prove (incl. 33 Coq theorems Coq for 15 000 lines)

Done with F. Clément, J.-C. Filliâtre, M. Mayero, G. Melquiond, P. Weis

$\Rightarrow$ now what?

Outline

Motivations

http://www.ima.umn.edu/~arnold/disasters/sleipner.html

The sinking of the Sleipner A offshore platform

Excerpted from a report of SINTEF, Civil and Environmental Engineering:

The Sleipner A platform produces oil and gas in the North Sea and is supported on the seabed at a water depth of 82 m. It is a Condeep type platform with a concrete gravity base structure consisting of 24 cells and with a total base area of 16 000 m^2. Four cells are elongated to shafts supporting the platform deck. The first concrete base structure for Sleipner A sprang a leak and sank under a controlled ballasting operation during preparation for deck mating in Gandsfjorden outside Stavanger, Norway on 23 August 1991.

Immediately after the accident, the owner of the platform, Statoil, a Norwegian oil company appointed an investigation group, and SINTEF was contracted to be the technical advisor for this group.

The investigation into the accident is described in 16 reports...

The conclusion of the investigation was that the loss was caused by a failure in a cell wall, resulting in a serious crack and a leakage that the pumps were not able to cope with. The wall failed as a result of a combination of a serious error in the finite element analysis and insufficient anchorage of the reinforcement in a critical zone.

A better idea of what was involved can be obtained from this photo and sketch of the platform. The top deck weighs 57,000 tons, and provides accommodation for about 200 people and support for drilling equipment weighing about 40,000 tons. When the first model sank in August 1991, the crash

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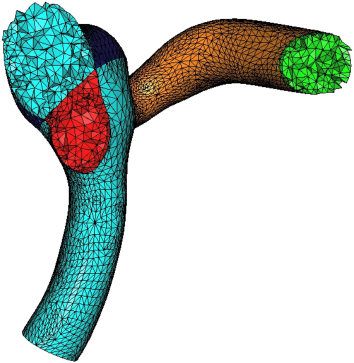

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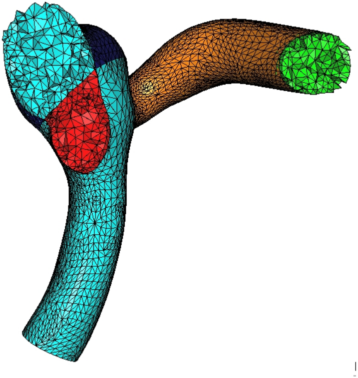

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Instead of regular 2D/3D grids, we consider meshes made of triangles/tetrahedra.

Motivations

The Finite Element Method (FEM) is the most used method to solve PDEs over meshes.

> *FEM encompasses methods for connecting many simple element equations over many small subdomains, named finite elements, to approximate a more complex equation over a larger domain.*
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First, let us understand/formally prove the mathematics.

Outline

Lax-Milgram?

- considered as the foremost theorem for the correctness of the Finite Element Method. (stating in a few slides)
- means that the (method) error may bounded when approximating an infinite-dimensional space by a finite-dimensional one.

  Example: functions and polynomials.

How to attack non-trivial mathematics?

Mathematicians at work for Lax-Milgram theorem

- more 50 pages of mathematical proofs

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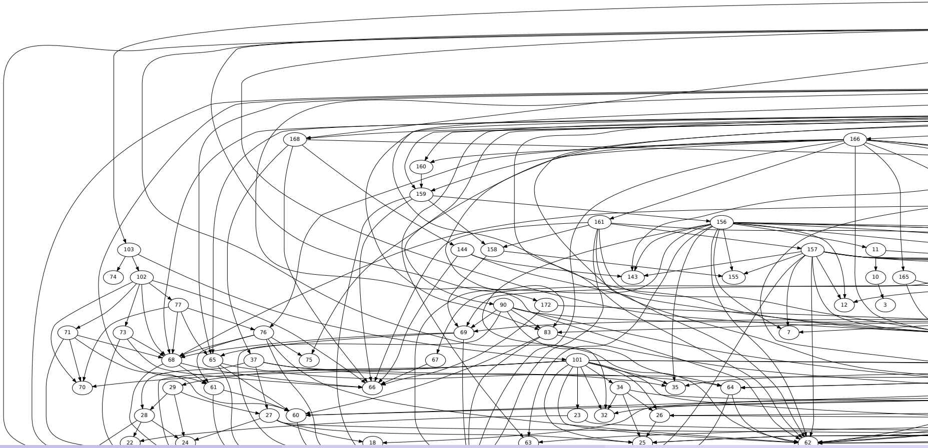

Proof engineering

Let us build upon the Coquelicot library (Boldo, Lelay, Melquiond)

+ general spaces

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+ general spaces
+ many existing theorems

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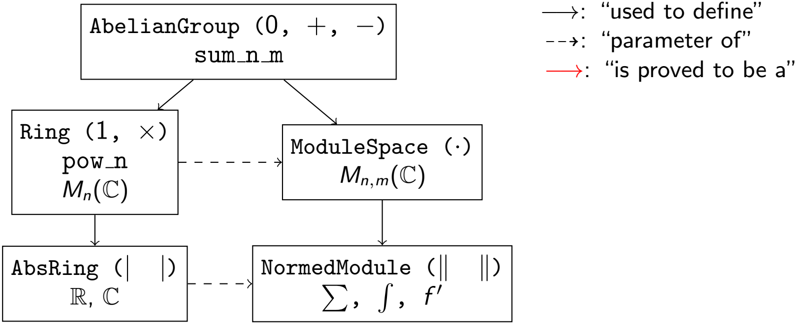
Let us build upon the Coquelicot library (Boldo, Lelay, Melquiond)

+ general spaces
+ many existing theorems
- not always the space we need

Enriched Hierarchy



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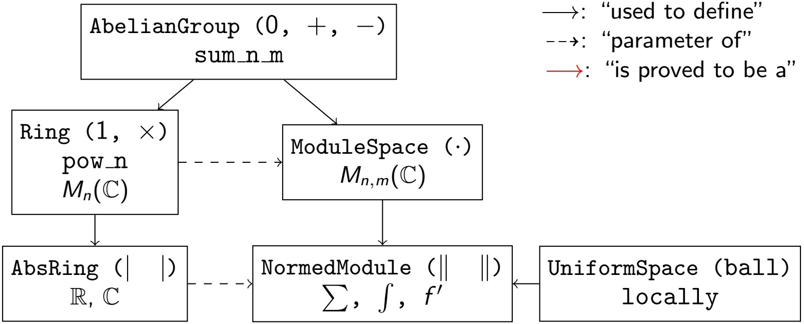

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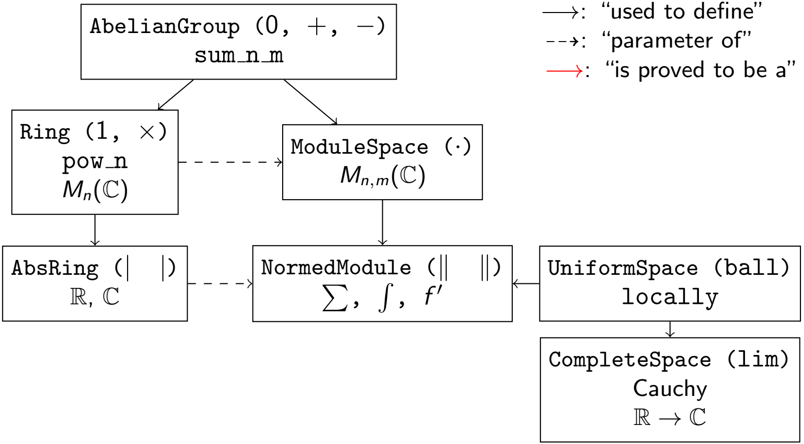

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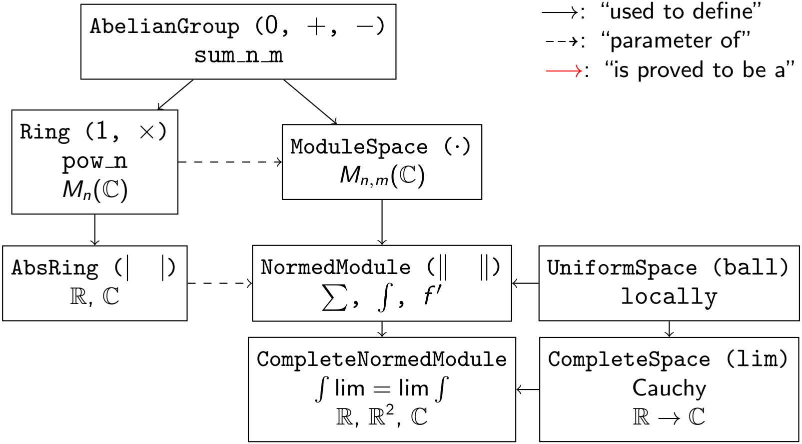

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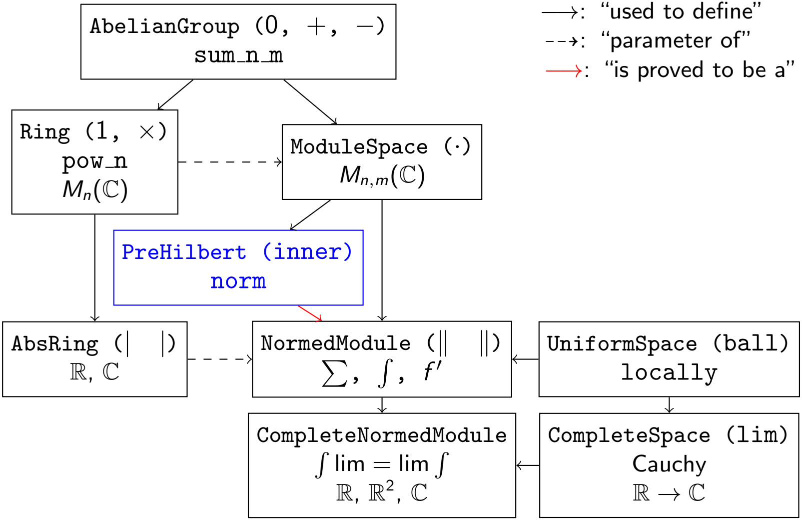

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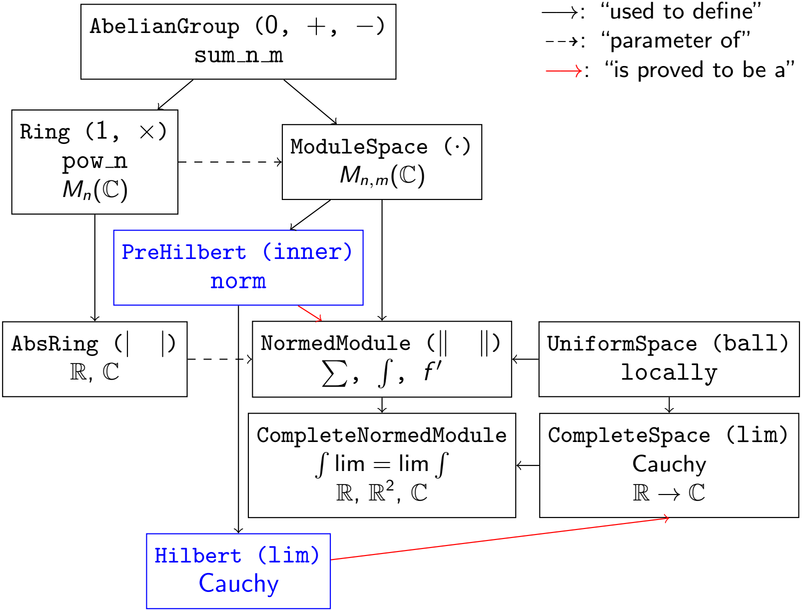

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- results about functional spaces, linear and bilinear mappings

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- prove Lax-Milgram theorem and Céa's lemma

Lax-Milgram Theorem and Céa's Lemma

Theorem (Lax-Milgram)

Let E : `Hilbert`, $f \in E'$, $C, \alpha \in \mathbb{R}_+^*$. Let $\varphi : E \to$ `Prop`, φ `ModuleSpace`-compatible and complete. Let a be a bilinear form of E bounded by C and α-coercive. Then:

$$\exists! u \in E, \varphi(u) \wedge \forall v \in E, \varphi(v) \Longrightarrow f(v) = a(u, v) \wedge \|u\|_E \leq \frac{1}{\alpha} |||f|||_\varphi.$$

Lemma (Céa)

Let E : `Hilbert`, $f \in E'$, $0 < \alpha$. Let $\varphi : E \to$ `Prop`, φ `ModuleSpace`-compatible and complete. Let a be a bilinear form of E, bounded by $C > 0$ and α-coercive. Let u and u_φ be the solutions given by Lax–Milgram Theorem respectively on E and on the subspace φ. Then:

$$\forall v_\varphi \in E, \varphi(v_\varphi) \Longrightarrow \|u - u_\varphi\|_E \leq \frac{C}{\alpha} \|u - v_\varphi\|_E.$$

Outline

Lax-Milgram Theorem in constructive logic

The first version of this theorem was:

$\mathcal{H}_1 = (\texttt{phi} : \texttt{E} \to \texttt{Prop}) : \texttt{forall u} : \texttt{E}, \texttt{forall eps} : \texttt{posreal},$
$\quad \texttt{decidable} (\texttt{exists w} : \texttt{E}, \texttt{phi w} \wedge \texttt{norm (minus u w)} < \texttt{eps}).$

$\mathcal{H}_2 = (\texttt{phi} : \texttt{E} \to \texttt{Prop}) (\texttt{f} : \texttt{topo\_dual E}) :$
$\quad \texttt{decidable} (\texttt{exists u}, \neg \neg \texttt{phi u} \wedge \texttt{f u} \neq 0).$

Theorem (Lax-Milgram)

Let $f \in E'$, $0 < \alpha$. Let $\varphi : E \to \texttt{Prop}$, φ `ModuleSpace`-compatible and complete. Let a be a bilinear form on E, bounded and α-coercive.
Suppose $\forall f \in E', \ \mathcal{H}_1(\ker(f) \ \wedge \ \neg\neg\varphi) \ \wedge \ \mathcal{H}_2(\varphi, f)$.
Then, there exists a unique $u \in E$ such that $\neg\neg\varphi(u)$ and

$$\forall v \in E, \quad \neg\neg\varphi(v) \implies f(v) = a(u, v) \quad \wedge \quad \|u\|_E \leq \frac{1}{\alpha} \cdot |||f|||_{\varphi}.$$

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Given the previous experiment, we added the excluded middle, both for readability and for spreading formal methods to mathematicians.

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(All this may hurt you, but mathematicians do that all the time.)

Back to the FEM

Towards the Coq formalization of the finite element method:

- Lax-Milgram theorem (✓)

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Outline

Measurability

Given a set `E→ Prop`, is it measurable?

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We chose the definition from the generator sets:

```
Context {E : Type}.

(* initialization sets *)
Variable gen : (E → Prop) → Prop.

Inductive measurable : (E→ Prop) → Prop :=
  | measurable_gen : forall omega, gen omega → measurable omega
  | measurable_empty : measurable (fun _ ⇒ False)
  | measurable_compl : forall omega,
        measurable (fun x ⇒ not (omega x)) → measurable omega
  | measurable_union_countable :
   forall omega:nat → (E→ Prop),
     (forall n, measurable (omega n)) →
        measurable (fun x ⇒ exists n, omega n x).
```

The measurable sets are aka σ-algebras.

Measurability

Advantages of `Inductive`:
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$\Rightarrow$ easy theorems

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We defined generators on $\mathbb{R}$ and $\overline{\mathbb{R}}$:

```
Definition gen_R_cc := (fun om ⇒ exists a b, (forall x, om x ↔ a <= x <= b)).
Definition gen_Rbar_mc := (fun om ⇒ exists a, (forall x, om x ↔ Rbar_le a x)).
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But we may use other generators and prove the measurable sets are the same. For instance `a` $<$ `x` $<$ `b` or with `a` and `b` in $\mathbb{Q}$.

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But we may use other generators and prove the measurable sets are the same. For instance `a < x < b` or with `a` and `b` in $\mathbb{Q}$.

And we proved that it is equivalent to the usual Borel σ-algebras:

```
Lemma measurable_R_open : forall om,
  measurable gen_R_cc om ↔ measurable open om.
```

Measurable functions

A function $f : E \to F$ is measurable if the set $A(f(x))$ is measurable in F for all measurable sets A in E:

```
Definition measurable_fun : (E → F) → Prop :=
  fun f ⇒ (forall (A: F → Prop), measurable genF A →
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The sum and multiplication by a scalar of measurable functions on $\mathbb{R}$ and $\overline{\mathbb{R}}$ are measurable functions.

Measure definition

We choose to not (yet) define the Lebesgue measure, but define what a measure is supposed to satisfy:

```
Context {E : Type}.
Variable gen : (E → Prop) → Prop.

Record measure := mk_measure {
   meas :> (E→ Prop) → Rbar ;
   meas_False : meas (fun _ ⇒ False) = 0 ;
   meas_ge_0: forall om, Rbar_le 0 (meas om) ;
   meas_sigma_additivity : forall omega :nat → (E→ Prop),
     (forall n, measurable gen (omega n)) →
     (forall n m x, omega n x → omega m x → n = m)
     → meas (fun x ⇒ exists n, omega n x)
             = Sup_seq (fun n ⇒ sum_Rbar n (fun m ⇒ meas (omega m)))
}.
```

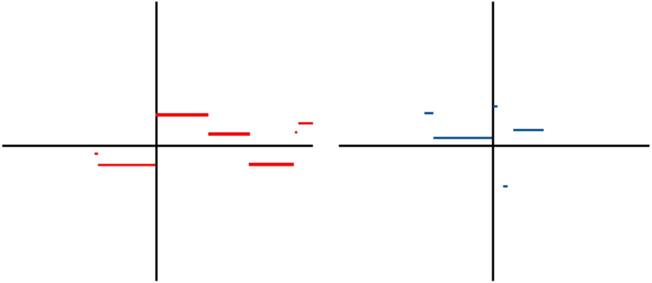
Measure properties

Many properties hold for all measures such as:

```
Lemma measure_Boole_ineq : forall (mu:measure) (A:nat → E→ Prop) (N : nat),
    (forall n, n <= N → measurable gen (A n)) →
      Rbar_le (mu (fun x ⇒ exists n, n <= N ∧ A n x))
              (sum_Rbar N (fun m ⇒ mu (A m))).
```

$$\mu\left(\bigcup_{i\in[0..N]} A_i\right) \leq \sum_{i\in[0..N]} \mu(A_i)$$

Simple functions?



Examples of simple functions @ mathonline

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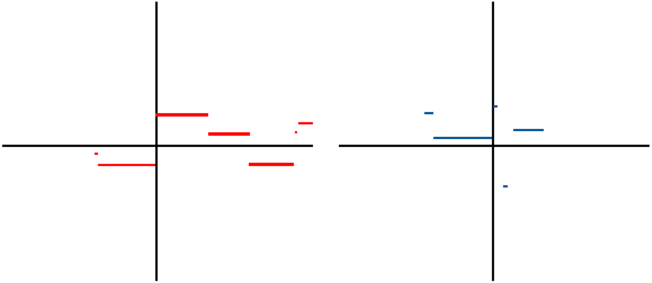

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We have tried various definitions of simple functions, especially as we prefer to sum over a finite set of values.

Simple functions definition

```
Definition finite_vals : (E→ R) → (list R) → Prop :=
    fun f l ⇒ forall y, In (f y) l.
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```
Definition finite_vals_canonic : (E→ R) → (list R) → Prop :=
  fun f l ⇒ (LocallySorted Rlt l) ∧
             (forall x, In x l → exists y, f y = x) ∧
             (forall y, In (f y) l).
```

⇒ unique!
We were able to construct the second list from the first.

Simple functions integration

$$\int f \, d\mu \overset{\text{def.}}{=} \sum_{a \in f(X)} a \, \mu\left(f^{-1}(a)\right) \quad \in \overline{\mathbb{R}}$$

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```
Definition SF_aux : (E→ R) → (list R) → Prop :=
  fun f l ⇒ finite_vals_canonic f l ∧
   (forall a, measurable gen (fun x ⇒ f x = a)).

Definition SF : (E→ R) → Set := fun f ⇒ { l | SF_aux f l}.

Definition af1 (f:E→ R) :=
  (fun a :  Rbar ⇒ Rbar_mult a (mu (fun (x:E) ⇒ f x = a))).

Definition LInt_simple_fun_p :=
   fun (f:E→ R) (H:SF gen f) ⇒ let l:= (proj1_sig H) in
     sum_Rbar_map l (af1 f).
```

We proved the value does not depends on the proof `H`.

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⇒ theorems about sum, multiplication by a scalar and change of variable

Lebesgue integral

$$\int f \, d\mu \stackrel{\text{def.}}{=} \sup_{\varphi \in \mathcal{SF}_+, \varphi \leq f} \int \varphi \, d\mu \quad \in \overline{\mathbb{R}}$$

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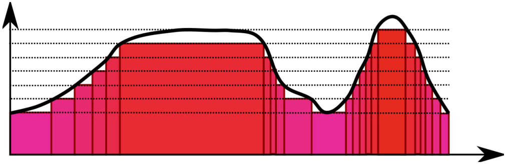

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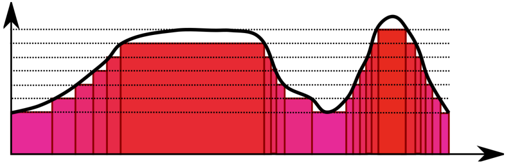
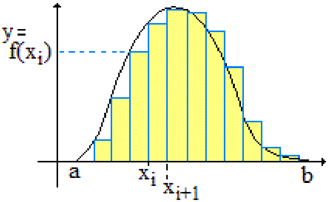
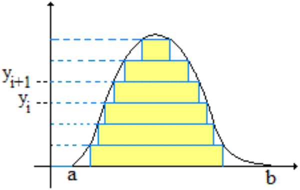




Riemann integral *vs* Lebesgue integral



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Lebesgue integral definition

$$\int f \, d\mu \stackrel{\text{def.}}{=} \sup_{\varphi \in \mathcal{SF}_+, \varphi \leq f} \int \varphi \, d\mu \quad \in \overline{\mathbb{R}}$$

```
Definition LInt_p :(E→ Rbar) → Rbar := fun f ⇒
     Rbar_lub (fun x ⇒ exists (g:E→ R), exists (Hg: SF gen g),
                      non_neg g ∧
                      (forall (z:E), Rbar_le (g z) (f z)) ∧
                      LInt_simple_fun_p mu g Hg = x).
```

A monotone convergence theorem

Theorem (Beppo Levi, monotone convergence)

Let $(f_n)_{n\in\mathbb{N}} \in \mathcal{M}_+$ be a sequence of nonnegative measurable functions, that is pointwise nondecreasing. Then, the pointwise limit of $(f_n)_{n\in\mathbb{N}}$ is nonnegative and measurable, and we have in $\overline{\mathbb{R}}$

$$\int \lim_{n\to\infty} f_n \, d\mu = \lim_{n\to\infty} \int f_n \, d\mu.$$

Note that $\lim_{n\to\infty} f_n = \sup_{n\in\mathbb{N}} f_n$ and $\lim_{n\to\infty} \int f_n = \sup_{n\in\mathbb{N}} \int f_n$.

```
Lemma Beppo_Levi : ∀ f : nat → E → Rbar,
  (∀ n, non_neg (f n)) → (∀ n, measurable_fun_Rbar genE (f n)) →
  (∀ x n, Rbar_le (f n x) (f (S n) x)) →
  LInt_p μ (fun x ⇒ Sup_seq (fun n ⇒ f n x)) = Sup_seq (fun n ⇒ LInt_p μ (f n)).
```

Focus on a hard theorem

Focus on a hard theorem

$$\int (f+g) = \int f + \int g$$

```
Lemma LInt_p_plus : forall f g,
    non_neg f → non_neg g →
    measurable_fun_Rbar gen f → measurable_fun_Rbar gen g →
    LInt_p mu (fun x ⇒ Rbar_plus (f x) (g x))
        = Rbar_plus (LInt_p mu f) (LInt_p mu g).
```

Proof of $\int(f+g) = \int f + \int g$ (1/2)

It needs adapted sequences:

```
Definition is_adapted_seq (f:E→ Rbar) (phi:nat→ E→ R) :=
    (forall n, non_neg (phi n)) ∧
    (forall (x:E) n,  phi n x <= phi (S n) x) ∧
    (forall n, exists l, SF_aux gen (phi n) l) ∧
    (forall (x:E),  is_sup_seq (fun n ⇒ phi n x) (f x)).
```

as their limit gives the integral:

```
Lemma LInt_p_with_adapted_seq :
   forall f phi, is_adapted_seq f phi →
      is_sup_seq (fun n ⇒ LInt_p mu (phi n)) (LInt_p mu f).
```

Proof of $\int(f+g) = \int f + \int g$ (2/2)

Adapted sequences may be defined like that:

$$\forall x, \quad f_n(x) \stackrel{\text{def.}}{=} \begin{cases} \dfrac{\lfloor 2^n f(x) \rfloor}{2^n} & \text{when } f(x) < n, \\ n & \text{otherwise.} \end{cases}$$

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that may be written in Coq as:

```
Definition mk_adapted_seq (n:nat) (x:E) :=
  match (Rbar_le_lt_dec (INR n) (f x)) with
           | left _ ⇒ INR n
           | right _ ⇒ round radix2 (FIX_exp (−n)) Zfloor (f x)
  end.
```

relying on fixed-point arithmetic defined by the Flocq library!!

And then:

```
Lemma mk_adapted_seq_is_adapted_seq :
   is_adapted_seq f mk_adapted_seq.
```

Outline

Definition of a finite element (geometry and properties)

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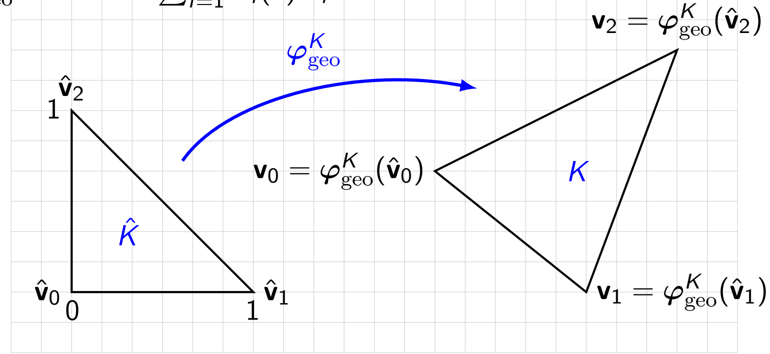
```
Record FE : Type := mk_FE {
  d : nat ; (* space dimension eg 1, 2, 3 *)
  ndof : nat ; (* nb of degrees of freedom - eg number of nodes for Lagrange.
  d_pos :    (0 < d)%coq_nat ;
  ndof_pos : (0 < ndof)%coq_nat ;
  g_family : geom_family ; (* either Simplex or Quad *)
  nvtx : nat := (* ... *) (* number of vertices *)
  vtx : '(' R^d)^nvtx ; (* vertices of geometrical element *)
  K_geom : 'R^d → Prop := convex_envelop vtx ; (* geometrical element *)
  P_approx : FRd d → Prop ; (* Subspace of F *)
  P_compat_fin : has_dim P_approx ndof ;
  sigma : '( FRd d → R)^ndof ;
  is_linear_mapping_sigma : forall i, is_linear_mapping (sigma i) ;
  FE _is_unisolvent :
       is_unisolvent d ndof P_approx P_compat_fin (gather sigma) ;
 }.
```

Geometrical transformation

Goal: to transform (and back) a finite element into a reference (nice) finite element.

$\varphi^K_{\mathrm{geo}} : \hat{K} \ni \hat{\mathbf{x}} \mapsto \sum_{i=1}^{n_V^K} \hat{\mathcal{L}}_i(\hat{\mathbf{x}})\, \mathbf{v}_i$ affine



Lagrange nodes

We want to define the simplest finite elements (Lagrange finite elements).

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Given d and k, I want the list of the vectors of $\mathbb{N}^d$ such that their sum is smaller than k (Lagrange nodes).

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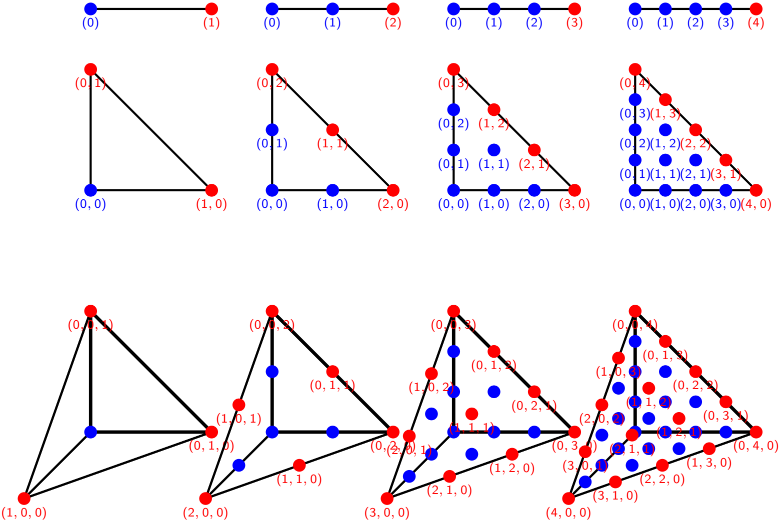
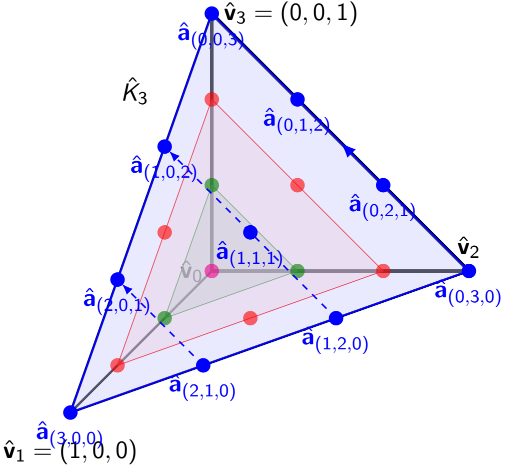
- or analysis?

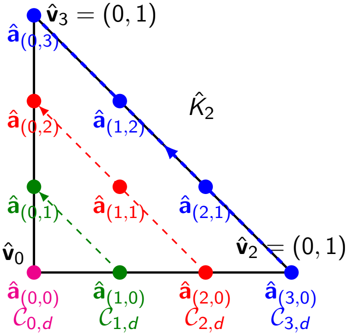
  Such a vector can be seen as a monomial among the polynomials on d variables of degree $\leq k$.

For $d = 1, 2, 3$ (in line) and $k = 1, 2, 3, 4$ (in column).



Construction of Lagrange finite element nodes





Coq formalization

We defined this list of vectors $\mathcal{A}_d^k$ (of size the binomial coefficient C_{d+k}^d) by concatenation of lists of varying sizes.

```
Lemma A_d_k_sum : forall d k i,
    (sum (A_d_k d k i) <= k)%coq_nat.

Lemma A_d_k_surj : forall d k (b:'nat^d),
    (sum b <= k)%coq_nat → exists i, b = A_d_k d k i.

Lemma A_d_k_inj : forall d k, injective (A_d_k d k).

Lemma A_d_k_MOn : forall d k, is_orderedF MOn (A_d_k d k).
    (* a special order near the grevlex order on monomials *)
```

Outline

Conclusion

A journey

- hand by hand with mathematicians,
- pretty long,
- with various mathematics inside.

Available at https://lipn.univ-paris13.fr/coq-num-analysis/
and as an opam package.

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Difficult parts:

- handling subspaces,
- trade-off between a usable library and proving one main theorem.

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- prove a real implementation (in floating-point arithmetic)

Thank you for your attention