Certification of Numerical Analysis Programs

(CerPAN-FOST)

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Framework

- Work in progress (supported by ANR)
- Numerical Problems
- Critical Programs
- Automated technics : transports, money, medicine, seismology, meteorology, ...
- Reliability of these technics : zero default programs, certification

Difficulties

- These methods are limited by numerical aspects of problems
- Sources of errors (computers, schemas, algorithms, humans,...)
- floating-point numbers
- Formal proofs of programs soundness :
  problems from continuum (vs discret world)
  - successor of float

Objectives

- To develop methods to formally prove correctness of programs from NA domain
- Programs which are often used to solve critical problems
- **NA** : methods can be useful to develop critical numerical programs
- **FP** : continue the development of proof systems with real numbers (floating-point numbers, exacts reals)
- Open these new technics to non experts users

Proofs of programs

- Why, Caduceus, Gappa
  - Why : software verification platform (general-purpose verification condition generator)
  - Caduceus : verif. tool for C programs ; built on top of Why.
  - Gappa : Génération Automatique de Preuves de Propriétés Arithmétiques. Tool intended to help verifying and formally proving properties on programs dealing with fp.
- Existing programs
- Annotations
- Proof Obligations (Coq,...)

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1. To deal with floating-point numbers
2. Case study
3. Automation

Different kinds of error

Computing errors (due to computers) :

- round errors : $(1 + 2^{-53}) - 1 = 0$
- representation errors : $\frac{1}{10}$
- exceptional behavior : NaN $(+\infty - \infty)$

Extraction

- Formal formalization of the problem
- Proofs
- Extraction : program proved to be correct

Extraction

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- Proofs
- Extraction : program proved to be correct

1. To deal with real numbers (which one ?)
2. Case study
3. Automation
4. Efficiency

Different kinds of error

Method error (known by the programmer and controlled) :

It is the intrinsic error due to the algorithm with respect to the exact mathematical value :

- cut series ($\sum_{i=0}^{N} a_i$ instead of $\sum_{i=0}^{+\infty} a_i$)
- approximations ($1 + x + \frac{x^2}{2}$ for $\exp(x)$)
- neglect some terms
- ...

To bound errors

- To bound the computing error :
  If $|x| \leqslant 2^{-3}$, then $|y - (1 + x + \frac{x^2}{2})| \leqslant 2^{-52}$
- To bound the computing error and the method error :
  If $|x| \leqslant 2^{-3}$, then $|y - exp(x)| \leqslant 2^{-51}$
- To bound all errors (x is an approximation of X) :
  If $|X| \leqslant 2^{-3}$ and $|X - x| \leqslant 2^{-50}$, then
  $|y - (1 + X + \frac{X^2}{2})| \leqslant 2^{-48}$

Case study

The analytic gradient :

Minimization of function $J(P) = \frac{1}{2}||d - F(P)||^2$
where d is an experimental measure and $F(P)$ is the theoretical function
$\Rightarrow grad(J(P)) = 0$

Case study

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Decomposition into two parts :

1. Resolution of the partial differentiation equation thanks to a numerical schema
   $\longrightarrow$ Proof of schema stability
2. Computing of the derivative of a simple function :
   square of Euclidian norm on $\mathbb{R}^n$

Methodology

- Proof of program
- Caduceus
- Calculus error
- Floating-point numbers

The floating-point model inside Caduceus

```
Flottant Why (x) =
    flottant : x
    real : x@1
    real : x@2
```

- `x` is the value of the **floating-point number** in memory
- `x@1` is the **value** if all calculus would have been exacts
- `x@2` is the **ideal** result (including measure errors)

Examples of annotations

- ```
  /* @ requires |x|<=2^(-3)
     @ ensures |\result - \result@1| <= 2^(-52) */
  ```
- ```
  /* @ requires |x|<=2^(-3)
     @ set \result@1=exp(x@1)
     @ ensures |\result - \result@1| <= 2^(-51) */
  ```
- ```
  /* @ requires |x@2|<=2^(-3) and |x-x@2|<=2^(-50)
     @ set \result@2=exp(x@2)
     @ ensures |\result - \result@2| <= 2^(-48) */
  ```
  ```

Malcolm algorithm (1/2)

Annotated program :

```
/*@ logic int my_log(real s) */
/*@ ensures \result == 2 ^^ (53) */
double malcolm1() {
   double A;
   A=2;
   /*@ assert A==2 */
   /*@ invariant A== 2 ^^ my_log(A) && 1 <= my_log(A) <= 53
       variant (53-my_log(A)) */
   while (A != (A+1)) {
     A*=2;
   }
   return A;
}
```

Malcolm algorithm (2/2)

Proofs obligations :

```
(*Why goal*) Lemma malcolm1_impl_po_2 :
  forall (A: double),
  forall (HW_2: A = (r_to_d nearest_even (IZR 2))),
  forall (HW_3:
(* File "Malcolm.c", line 8, characters 14-18 *)
              (eq (d_to_r A) (IZR 2))),
(* File "Malcolm.c", line 10, characters 17-73 *)
  ((eq (d_to_r A) (Rpower (IZR 2)
        (IZR (my_log (d_to_r A))))) /\ 1 <=
  (my_log (d_to_r A)) /\ (my_log (d_to_r A)) <= 53).
...
```

Dirichlet

```
#include "dirichlet.h"
/*@ requires ni >= 2 && nk >= 2
             && 1 <= is < ni && 1 <= ir < ni
             && dx > 0. && dt > 0.
             && \valid_range(f,1,nk-1)
             && \valid_range(v,1,ni-1)
             && \forall int i; 1 <= i < ni => v[i] > 0.
             && \forall int i; 1 <= i < ni => v[i]*dt/dx < 1.
 */

double **forward_prop(int ni, int nk, int is, double dx,
     double dt, double *f, double *v) {
...
/*@ invariant 1 <= i <= ni variant ni-i */
...
```

Methodology

- Direct specification
- Coq
- "Algorithm error"
- Known by the programmer

Convergency

Wave equation :

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$$

$$u \underset{\longrightarrow}{?} u_h \text{ (approximated solution)}$$

$$\text{method error} \equiv \text{convergency}$$

$$\text{consistency } /\backslash \text{ stability} \longrightarrow \text{convergency}$$

Consistency

Explicit centered schema :

$$\varepsilon_j^n = \frac{u_h^{n+1} - 2u_h^n + u_h^{n-1}}{\Delta t^2} - c^2 \frac{u_{h+1}^n - 2u_h^n + u_{h-1}^n}{\Delta x^2}$$

2nd order consistency :

$$\varepsilon_j^n = O(\Delta t^2 + \Delta x^2)$$

Stability

Perturbative data : how is the solution changed ?

On a bounded time interval :

$$||u_h^n||_{L^2} \leq C(||u_0||_{L^2} + t^n||u_1||_{L^2})$$

Difficulties

- Consistency :
  - Definition of O
  - Imprecise notations (ex : $O(\Delta x^2 + \Delta t^2)$)
  - To swap quantifiers
  - Mixed time and space problems
  - Uniform Taylor series
- Stability :
  - 2 methods (at least) :
  - Fourier
  - Energetic technics

Conclusion

- Separated treatment of the 2 errors : floating-point and method error
- Addition of floating-point numbers into Caduceus
- Proof of floating-point error
- Addition of a new tactic “gappa” into Coq
- Specification of method error
- FOST (Formal proOfs of Scientific compuTation programs)