Modélisation et résolutions numérique et symbolique

via les logiciels Maple et Matlab

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Format du cours

Équipe pédagogique : Stef Graillat (responsable), Jeremy Berthomieu, Mohab Safey El Din

Évaluation des connaissances

- un examen réparti 1 (25%), un examen réparti 2 (60%) et une note de TD/TME (15%)
- 10 séances de TME (dont certains seront à rendre)

Horaire

- Cours : le jeudi de 13h30 à 15h30 (salle 23-24/102)
- TD/TME : le vendredi de 13h30 à 15h30 (salle 23-24/102) et de 15h45 à 17h45 (salle 31/313)

Site web :
`http://www-pequan.lip6.fr/~graillat/teach/model/index.html`

Objectives of the course

- Mathematical concepts in Computer Science : basic definitions
- Algorithms: on mathematical structure $\rightsquigarrow$ how to compute efficiently and reliably ?
- Problem solving : several models of resolution

Application fields

- cryptology
- data-mining
- signal theory and computer vision
- image rendering
- robotics
- computational geometry
- biology
- etc.

Symbolic computation/Numerical computation

Paradigms of solving:

- Global Approaches: Compute **all** the solutions and ensure the quality of the returned results.
- Local (iterative) Approaches: Compute an *approximation* of a local solution (in a prescribed domain) by iterating a certain function.

Example: Solve $f = 0$ where $f \in \mathbb{Q}[X]$

- "Compute" all the real roots (or the complex ones)
- Decide the existence of a real root
- Return an approximation "close" to a real root (or a complex one)

Family of algorithms:

- Symbolic Algorithms: provide an exact representation of the result but sometimes are slow $\rightsquigarrow$ Computer Algebra
  Cryptology, Error correcting codes, Comp. Geometry, classification problems

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  Numerical validation, Computer arithmetics, Numerical simulation

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$\rightarrow$ Hybrid symbolic-numeric computing : use both advantages of approaches

General outline of the course

1. Introduction to Maple
2. Rings, Fields, multi-precision and multi-modular arithmetic
3. Application to linear solving (Gauss paradigm) – Evaluation/Interpolation techniques
4. Euclid's paradigm and non-linear solving
5. Introduction to MATLAB
6. Singular Value Decomposition, application to image compression
7. Eigenvectors/eigenvalues and application to Google PageRank algorithm
8. Discrete Fourier Transform, application to signal theory
9. Monte-Carlo Methods, application to pricing option in finance

Bibliographie

- Maple, Règles et fonctions essentielles, N. Puech, Springer, 2009
- Maple Sugar: Une initiation progressive à Maple, G. Le Bris, Cassini, 1999
- Introduction to Maple, A. Heck, 3e édition, Springer, 2003
- Essential Maple 7: An Introduction for Scientific Programmers, R. Corless, Springer, 2002
- Maple and Mathematica: A Problem Solving Approach for Mathematics, I. Shingareva et C. Lizarraga-Celaya, Springer, 2007
- Maple - Son bon usage en mathématiques, Ph. Dumas et X. Gourdon, Springer, 1997

General overview of Maple

- Software widely used in industry, research centers and for teaching
- Acronym for "MAthematical PLEasure"
- Initially, it was developped at the Univ. of Waterloo (Ontario, Canada).
  Then it became a product of Waterloo Maple Software Corporation.
  Bought by Toyota in 2010.

General overview of Maple

Advantages :

- computer algebra software
- interactivité/interface pratique :
  - programmation rapide et simple, facilité pour tester et modifier
  - oubli du bas niveau ; on se consacre pleinement à l'aspect algorithmique
- riche en fonctionnalités
- prises en compte des notions mathématiques formelles
- retourne des résultats sous la forme d'objets mathématiques
- permet l'interfacage avec des codes C et C++ (librairie dynamique)

Disadvantages :

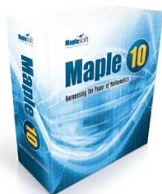
- pas de notion de compilation, peu d'entrées/sorties
- sémantique du langage pas toujours claire

Lancement de Maple

Le nom du fichier exécutable est

- `maple`, en mode texte
- `xmaple`, avec interface graphique
  plus légère avec l'option `-cw` (classic worksheet).

Sur les machines de l'ARI, il s'agit de Maple 10. Le programme est situe dans le répertoire `/usr/local/maple10/bin`



Quelques points de syntaxe

- L'instruction `quit` permet de quitter une session Maple
- L'aide sur une fonction, un type, . . . s'appelle par l'instruction `?` suivi du mot concerné. Par exemple `?string`
- Une instruction se termine par un point-virgule ; (sauf l'aide et quit) ou un double point :
  Le point-virgule ; permet d'exécuter la commande et d'afficher le résultat. Si l'on veut simplement exécuter les commandes sans voir le résultat s'afficher, il faut remplacer le point-virgule par deux points :
- Touche `Entree` $\rightarrow$ Exécution
- Commentaires : après un dièse #
- La commande `restart` remet tout dans l'état initial (annule toutes les définitions). Cela devrait être la première instruction de tout programme Maple

Quelques points de syntaxe

Le symbole > représente le prompt. Plusieurs instructions peuvent être regroupées sous un même prompt : elles forment un bloc d'instructions. Les instructions formant un bloc seront exécutées à l'aide d'une seule validation (par la touche `Entree`). Pour entrer plusieurs commandes dans le même bloc d'instructions, il suffit de taper `Maj` puis `Entree`

Il faut noter que Maple respecte la casse des lettres c'est-à-dire fait la différence entre majuscules et minuscules.

Il est aussi possible **(fortement recommandé)** d'écrire des scripts Maple (fichiers texte) dont l'exécution est lancée par `read "nom_fichier";` (utile pour écrire de gros codes).

Alternative

```
if cond1 then
   instructions1
else
   instructions2
fi
```

Si plusieurs alternatives imbriquées

```
if cond1 then
   instructions1
elif cond2 then
   instructions2
else
   instructions3
fi
```

Boucle for

```
for var from expIni to expFin do
   instructions
od;
```

Changer le pas de la variable de boucle

```
for var from expIni to expFin by pas do
   instructions
od;
```

Boucle Tant que

```
while expr do
   instructions
od;
```

Fonctions et procédures

Définition par le mot-clef `proc`

Syntaxe :
Le mot-clef `proc` permet de définir une fonction en respectant la syntaxe suivante :

```
MAFONCTION:=proc( param )
   d\'eclarations optionnelles
   corps de la fonction
end
```

Puis

```
MAFONCTION(param);
```

Visibilité des variables

Variable globale : variable présente dans l'environnement d'exécution jusqu'à la fin de la session

- Déclaration explicite : Mot clef `global`
- Déclaration explicite d'une variable globale à l'intérieur d'une fonction: dans la partie "déclarations optionnelles", par

  ```
  global s\'equence_des_variables_globales
  ```

Variable locale : variable qui n'est accessible qu'à l'intérieur d'une fonction. Elle ne vit que le temps d'exécution de cette fonction.

L'espace mémoire qui lui est alloué est libéré à la fin de l'exécution de la fonction.

- Déclaration explicite : mot clef `local`
- Déclaration explicite par

  ```
  local s\'equence_variables_locales
  ```

Exemple de fonctions

```
fibo:= proc(n)
if n<=1 then return 1;
else return fibo(n-1)+fibo(n-2);
end:
```

```
toto:=proc(n)
  local res;
  res:=1;
  for i from 1 to n do
    res:=res*i;
  od;
end;
```

```
foo:=proc(a, b)
if a=b then return a;
else
   if a>=b then return foo(a-b, b);
   else return foo(b-a, a);
   fi;
end;
```

Entiers, rationnels, flottants, complexes

- Maple peut gérer des entiers jusqu'à 500000 chiffres décimaux

```
> N := 100!;
N := 9332621544394415268169923885626670049071596826438
     16214685929638952175999932299156089414639761565182
     86253697920827223758251185210916864000000000000000
     000000000
```

- Maple simplifie systématiquement les rationnels

```
> x := 1/21 + 3/35;
                        x := 2/15
```

- La précision des nombres flottants est contrôlée par la variable `Digits`. Par défaut, `Digits` vaut 10

```
> 1.2^20;
                        38.33759992

> Digits:=20: 1.2^20;
                        38.337599924474751222
```

Entiers, rationnels, flottants, complexes (suite)

- On peut évaluer une expression en flottant par la commande `evalf`

```
> Digits:=30 : x:=exp(Pi*sqrt(163)); evalf(x);
                                        1/2
                    x := exp(Pi 163    )
                                                          18
                    0.262537412640768744000000000024 10
```

- Le nombre complexe $i = \sqrt{-1}$ est représenté par `I` en Maple

```
> z:=(1+2*I)^2;
                    z := -3 + 4 I
```

- Pour mettre un complexe sous forme cartésienne, on utilise `evalc`

```
> z^(1/2);
                                   1/2
                    (-3 + 4 I)
> evalc(%);
                    1 + 2 I
```

Entiers, rationnels, flottants, complexes (suite)

`iquo(m,n)`	quotient de la division euclidienne de m par n
`irem(m,n)`	reste de la division euclidienne de m par n
`ifactor(n)`	factorisation de l'entier n
`numer`, `denom`	numérateur et dénominateur d'une fraction
`trunc`, `round`, `frac`, `floor`, `ceil`	parties entières ou fractionnaire
`evalf`	évaluation numérique en flottant
`evalc`	évaluation d'un complexe

Some abstaction

All algorithms run over domains (sets of objects) that share arithmetic operations.

Abstracting these domains, i.e. identifying the properties satisfied/required by these domains allows to

- Introduce some genericity in programming;
- Extend computational paradigms/algorithms designed in "simple" domains to more sophisticated ones.

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Our roadmap

- We will define abstract domains rings and fields and relate them to sets of numbers.
- We will review some well-known computational paradigms in this context.
- We will extend them to more sophisticated rings and fields (e.g. the polynomial world)

Rings

A ring is a set R equipped with a $+$ and a $\times$ where everything happens as expected.

Addition and substraction

- $a - a = 0$
- $a + b = b + a$
- $a + (b + c) = (a + b) + c$

Multiplication

- $a \times (b \times c) = (a \times b) \times c$

Multiplication and Addition

- $a \times (b + c) = a \times b + a \times c$

and

- there exists $\mathbf{0} \in R$ such that, for all $a \in R$, $a + \mathbf{0} = a$;
- for all $a \in R$, there exists b such that $a + b = \mathbf{0}$;
- there exists an element $\mathbf{1} \in R$such that, for all $a \in R$, $\mathbf{1} \times a = a$

Examples (and non-examples) of rings

Examples integers, rationals, reals, complex numbers

Counter-example The set of (machine) floats is not a ring !

```
void main(){
  float a, b, c;
  a = 3432.675;
  b = 0.03232;
  c = 24.535;
  printf("%f\n", ((a+b)+c) - (a+(b+c)));
}
```

-0.000244

Subsidiary question: is the set of even odd integers a ring?

A bit more sophisticated example

Bits with xor $(+)$ and and $(\times)$ form a ring

$+$	0	1
0	0	1
1	1	0

and

$\times$	0	1
0	0	0
1	0	1

Rule Do operations over the integers and reduce modulo 2

Notation $\{0,1\} = \mathbb{F}_2 = \frac{\mathbb{Z}}{2\mathbb{Z}}$

Back to integers

Representation (base 2) $n = a_0 + a_1 2 + a_2 2^2 + \cdots + a_P 2^P$ with $a_i \in \{0, 1\} = \mathbb{F}_2 = \frac{\mathbb{Z}}{2\mathbb{Z}}$ (with $a_P \neq 0$)

Size of an integer

- We expect it to be the size of the array $a_0, \ldots, a_P$
- In base 2: size$(n) = \simeq \lceil \log_2(n) \rceil$
- In base B: $\simeq \lceil \log_B(n) \rceil$ (size in base 2 multiplied by a constant)

Bit complexity counts the number of operations of single/bit operations $\rightarrow$ takes into account growth of coefficients

Complexity of basic operations

Assuming $\tau = \text{size}(n) \geq \text{size}(m)$,

Addition of n, m in $O(\text{size}(n))$

Multiplication of n, m:

$$\mathsf{M}_{\text{int}}(\tau) \in O(\tau^2)$$

(naive)

$$\mathsf{M}_{\text{int}}(\tau) \in O(\tau^{1.59})$$

(Karatsuba)

$$\mathsf{M}_{\text{int}}(\tau) \in O(\tau \log \tau \log \log \tau)$$

(Fast Fourier Transform)

Quotients and remainders

Let A and B be two integers. The quotient and remainder are defined through

$$A = BQ + R$$

with

$$0 \leq R \leq |B|.$$

Notation: $Q = A \text{ div } B$ and $R = A \text{ rem } B$

Complexity Assuming that $\text{size}(A) = \tau \geq \text{size}(B)$,

- $O(\tau^2)$ bit operations (naive)
- $O(\mathsf{M}_{\text{int}}(\tau))$ bit operations (Newton, not in this course)

GCD and Euclide's algorithm

Let A and B be two integers. The greatest common divisor (GCD) of A, B is the greatest non-negative integer G dividing both A and B.

Some immediate relations

- $\mathrm{GCD}(A, B) = \mathrm{GCD}(B, A)$
- if $A \geq B$, $\mathrm{GCD}(A, B) = \mathrm{GCD}(A - B, B)$
- $\mathrm{GCD}(CA, CB) = C\,\mathrm{GCD}(A, B)$

GCD and Euclide's algorithm

Input: A, B integers
Output: R and U, V such that $R = \text{GCD}(A, B)$ and $R = AU + BV$
Q, RS, US, VS are local variables which will store intermediate datas
Equations $R = AU + BV$ and $R' = AU' + BV'$ are loop invariants

```
#Initialize :
R := A, R' := B, U := 1, V := 0, U' := 0, V' := 1
while (R' <> 0) do
    Q := iquo(r, r');
    RS := R, US := U, VS := V;
    R := R', U := U', V := V';
    R' := RS - Q *R', U' = US - Q*U', V' = VS - Q*V';
od;
return R, U, V;
```

Complexity is in $O(\text{size}(A)^2)$ (assuming $A \geq B$) – Proof is skipped.

Bézout relation

Let A and B be two integers and $G = \mathrm{GCD}(A, B)$.
There exist integers U and V such that

$$AU + BV = G$$

Some consequences

- If $G = 1$ (one says that A and B are coprime), there exist U and V such that $AU + BV = 1$
- Then, U is the inverse of A modulo B; in other words

$$AU \,\mathrm{rem}\, B = 1$$

Fields

A field is a set F with a $+$ and a $\times$ where everything happens as expected when one wants to use division.

- $(F, +, \times)$ is a ring
- for all $a \in F$ such that $a \neq 0$ there exists b such that

$$a \times b = 1$$

We write $b = a^{-1}$ and call it the inverse of a.

Examples of fields

Intuitive examples rationals, reals, complex numbers

Counter examples integers

Def. Let N be a positive integer.

$\frac{\mathbb{Z}}{N\mathbb{Z}} = \{0, 1, \ldots, N-1\}$ equipped with $\oplus$ and $\otimes$ such that

- for a, b in $\frac{\mathbb{Z}}{N\mathbb{Z}}$,
$$a \oplus b = (a + b) \text{ rem } N$$
- for a, b in $\frac{\mathbb{Z}}{N\mathbb{Z}}$,
$$a \otimes b = (a \times b) \text{ rem } N$$

Theorem If N is prime, then $\frac{\mathbb{Z}}{N\mathbb{Z}}$ is a field.

Multi-modular arithmetic

Some observations:

- Bit complexity analysis of algorithms will take into account coefficient growth during the whole computational process
- For some algorithms, it may be possible that the size of the output is smaller than the size of intermediate coefficients.
- Idea: compute the output "modulo" several prime numbers (e.g. in a field) $\rightarrow$ control of the size of the intermediate coefficients.

Chinese Remainder Theorem

Let $P_1, \ldots, P_k$ be pairwise coprimes and $A_1, \ldots, A_k$ be a sequence of integers such that $A_i \in \frac{\mathbb{Z}}{P_i\mathbb{Z}}$.

There exists an integer X such that

$$\begin{aligned} X &= A_1 \mod P_1 \\ &\vdots \\ X &= A_k \mod P_k \end{aligned}$$

Moreover, all solutions are congruent modulo $N = P_1 \cdots P_k$.

Application: Choose $P_1, \ldots, P_k$ prime of size smaller than the word machine.

Chinese Remainder Reconstruction (2 equations)

Let us focus on the case of 2 equations:

$$X = A_1 \mod P_1 \quad \text{and} \quad X = A_2 \mod P_2$$

- Since P_1, P_2 are co-prime, $\mathrm{GCD}(P_1, P_2) = 1$.
- By the Bézout relation, this implies that there exist U, V such that

$$UP_1 + VP_2 = 1.$$

- Consequently, for any X, the following holds:

$$XUP_1 + XVP_2 = X$$

.

Now, remark that

$$X \mod P_1 = XVP_2 \mod P_1 = X \times 1 \mod P_1$$

Thus, taking

$$X = A_1VP_2 + A_2UP_1$$

provides a solution.

Chinese Remainder Reconstruction

Take $P = P_1 \times \cdots \times P_k$.
For $1 \leq i \leq k$,

- remark that $\frac{P}{P_i}$ and P_i are co-prime.
- take U_i as the inverse of $\frac{P}{P_1}$ modulo P_i

$$U_i \frac{P}{P_i} + V P_i = 1$$

Construct

$$X = A_1 \frac{P}{P_1} U_1 + \cdots + A_k \frac{P}{P_k} U_k$$

Examples

- Solve $X = 2 \mod 3$ and $X = 3 \mod 5$
- Solve $X = 1 \mod 2$ and $X = 2 \mod 3$ and $X = 3 \mod 5$