Numerical Methods

DE2, Spring 2010

Zhenyu Yang

http://www.cs.aaue.dk/~yang/course/NMbasis/NM2010.htm

1

Textbook

- Peter R. Turner,

"Guide to Sceintific Computing" (Second Edition), Macmillan Press LTD, 2000.

2

Content (I)

- MM1: Introduction to numerical methods and Matlab
- MM2: Approximate evaluation of functions
- MM3: Iterative solutions of equations
- MM4: Newton's iteration method
- MM5: Secant iteration method

3

Content (II)

- MM6: Lagrange interpolation method
- MM7:Spline interpolation methods
- MM8: Solutions to differential equations
- MM9: Runge-Kutta methods and multistep methods
- MM10: Systems of differential equations

4

MM1: Introduction to numerical methods and Matlab

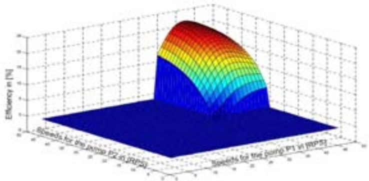
- Introduction
- Number representation and errors
- Matlab

5

Why do we need NM?

Machine computing

- Number representations (e.g., pi, 1.0000000123)
- Arithmetic calculation (e.g., 1/3, sqrt(2), e^2...)
- Algorithm development for solving complicated problems



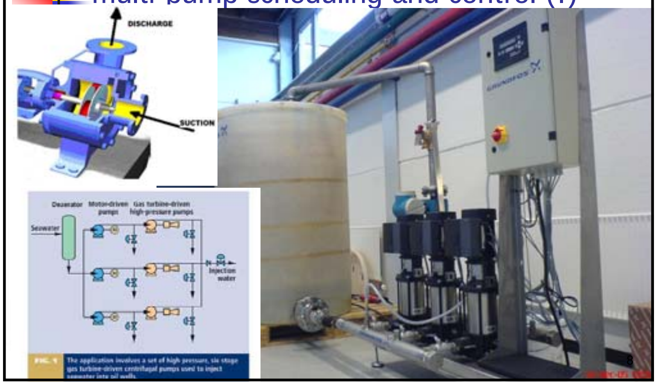
6

What does NM concern?

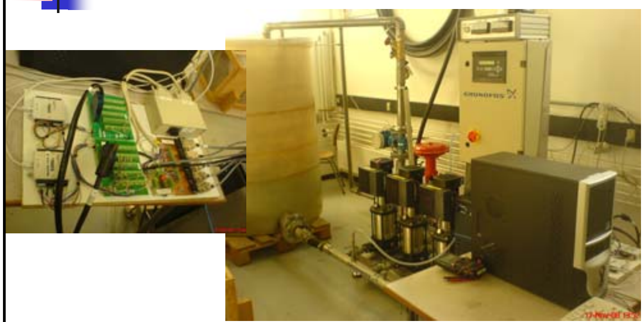
- Representation errors
- Accuracy
- Computation speed
- Required computation power
- Efficiency
- Robustness
- Robust, efficient computing algorithms with prescribed (acceptable) accuracy

7

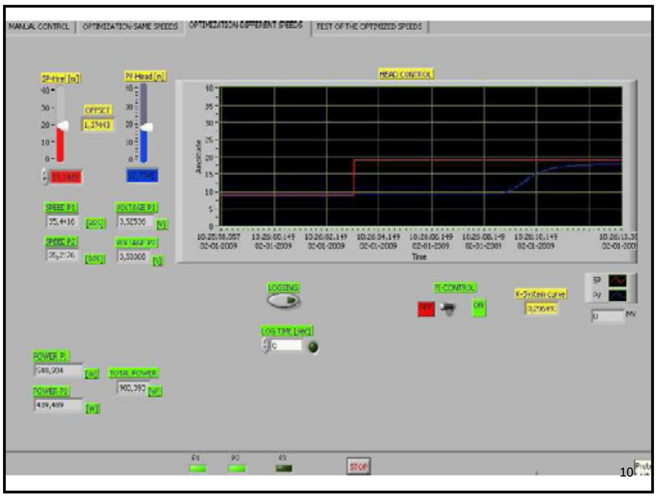
One practical example:
multi-pump scheduling and control (I)



One practical example:
multi-pump scheduling and control (II)



9

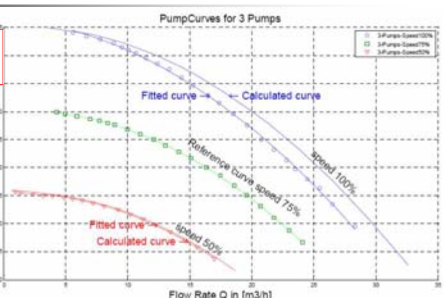


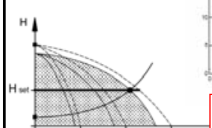
10

One practical example:
multi-pump scheduling and control (III)

$$H = \overline{a}_0 + \overline{a}_1 Q + \overline{a}_2 Q^2,$$
$$P = \overline{p}_0 + \overline{p}_1 Q + \overline{p}_2 Q^2 + \overline{p}_3 Q^3.$$

- Data acquisition
- Data analysis
- Interpolation
- Mathematical modeling





$$H_s(\omega) = a_0^s \omega^2 + a_1^s \omega Q_s(\omega) + a_2^s (Q_s(\omega))^2,$$
$$P_s(\omega) = p_0^s \omega^3 + p_1^s \omega^2 Q_s(\omega) + p_2^s \omega (Q_s(\omega))^2 + p_3^s (Q_s(\omega))^3$$

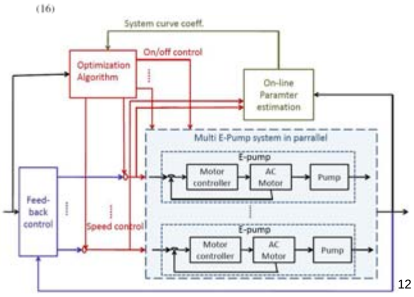
11

One practical example:
multi-pump scheduling and control (IV)

The optimization problem for N available pumps is defined as: *For a given demanded head and known system curve coefficients, find a number of available pumps, denoted as $i_1, \cdots, i_k$, which combination leads to*

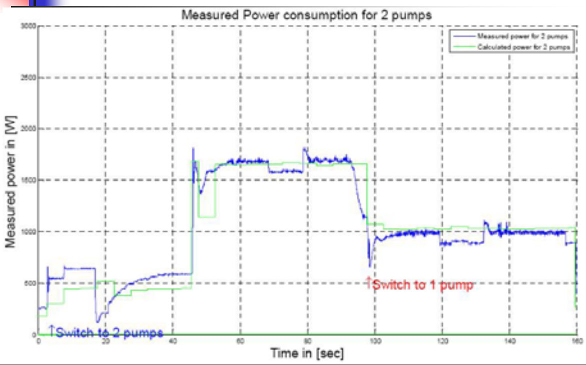
$$\max_{\substack{i_1,\cdots,i_k,\\ i_1,\cdots,i_k \in \{1,2,\cdots,N\}\\ \omega_{i_1},\cdots,\omega_{i_k}\\ 0 \le k \le N}} \eta_s(\varpi). \qquad (16)$$

- Constraint optimization
- Numerical solution
- Mixed integer nonlinear programming
- Lagrangian multipliers method
- Newton's mthod



12

One practical example:
multi-pump scheduling and control (V)

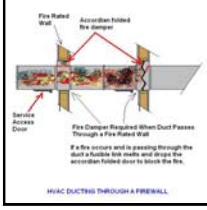


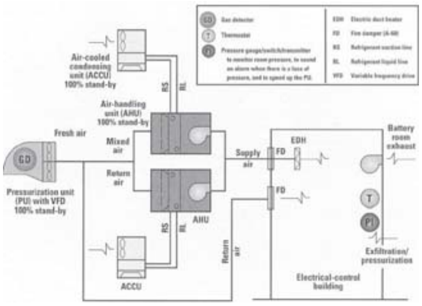
13

Practical example:
Control of offshore HVAC system (I)

14

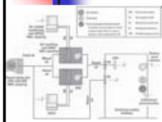
Practical example:
Control of offshore HVAC system (II)

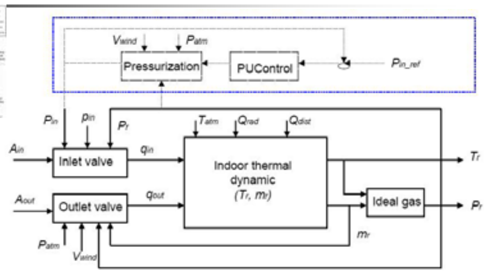




15

Practical example:
Control of offshore HVAC system (III)





$$C_{air} m_r \dot{T}_r = \dot{Q}_{rad} + \dot{Q}_{in} + \dot{Q}_{out} + \dot{Q}_{dis} + \dot{Q}_{dist},$$

$$q_{out} = c_{out} A_{out} \sqrt{\frac{2\Delta P_{out}}{\rho_r}}$$

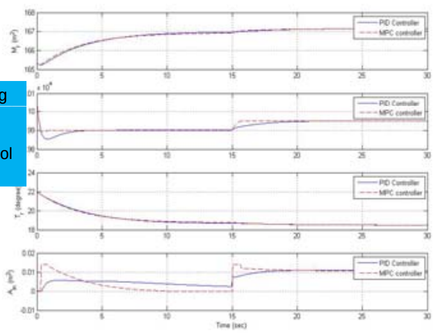
$$P_r = R_a \frac{m_r}{V_r} T_r$$

$$\dot{Q}_{in} = C_{air} \dot{m}_{in} (T_{in} - T_r)$$

16

Practical example:
Control of offshore HVAC system (IV)

- Mathematical modeling
- Simulation (Matlab) Differential equations
- Model predictive control (on-line optimization)



17

Introduction to Matlab....

>> demo

18

Number representation

- Range of numbers
- Accuracy of representation
- Fixed-point number
- Floating-point number
  - Numbers are in general represented approximately to a fixed number of significant digits and scaled using an exponent. The base for the scaling is normally 2, 10 or 16.
  - The typical number that can be represented exactly is of the form:

significant digits × *base*^{exponent}

19

Floating-point representation

- Base (radix):
  decimal (10), binary (2), hexadecimal (16)
- Mantissa (significant digits, significand)
- Exponent
- Normalization
- floating-point numbers achieve their greater range at the expense of precision.

20

IEEE 754 Standard

The IEEE has standardized the computer representation for binary floating-point numbers in IEEE 754. This standard is followed by almost all modern machines. Notable exceptions include IBM mainframes, which support IBM's own format (in addition to the IEEE 754 binary and decimal formats), and Cray vector machines, where the T90 series had an IEEE version, but the SV1 still uses Cray floating-point format.

$(-1)^s \times c \times b^q$
where b is the base (2 or 10). For example, if the sign is 1 (indicating negative), the significand is 12345, the exponent is −3, and the base is 10, then the value of the number is −12.345.

Name	Common name	Base	Digits	E min	E max	Notes
binary16	Half precision	2	10+1	-14	+15	storage, not basic
binary32	Single precision	2	23+1	-126	+127	
binary64	Double precision	2	52+1	-1022	+1023	
binary128	Quadruple precision	2	112+1	-16382	+16383	
decimal32		10	7	-95	+96	storage, not basic
decimal64		10	16	-383	+384	
decimal128		10	34	-6143	+6144	

21

Floating-point arithmetic

- Addition and subtraction

```
  123456.7 = 1.234567 * 10^5
  101.7654 = 1.017654 * 10^2 = 0.001017654 * 10^5
Hence:
123456.7 + 101.7654 = (1.234567 * 10^5) + (1.017654 * 10^2)
                    = (1.234567 * 10^5) + (0.001017654 * 10^5)
                    = (1.234567 + 0.001017654) * 10^5
                    =  1.235584654 * 10^5

   e=5;  s=1.235585    (final sum: 123558.5)
```

Note that the low 3 digits of the second operand (654) are essentially lost. This is round-off error. In extreme cases, the sum of two non-zero numbers may be equal to one of them:

22

Loss of significant Digits

Another problem of loss of significance occurs when two close numbers are subtracted. In the following example $e = 5$; $s = 1.234571$ and $e = 5$; $s = 1.234567$ are representations of the rationals 123457.1467 and 123456.659.

```
  e=5;  s=1.234571
- e=5;  s=1.234567
----------------
  e=5;  s=0.000004
  e=-1; s=4.000000 (after rounding/normalization)
```

The best representation of this difference is $e = -1$; $s = 4.877000$, which differs more than 20% from $e - -1$; $s - 4.000000$. In extreme cases, the final result may be zero even though an exact calculation may be several million. This *cancellation* illustrates the danger in assuming that all of the digits of a computed result are meaningful. Dealing with the consequences of these errors is a topic in numerical analysis; see also Accuracy problems.

23

Sources of errors

- Rounding errors
- Truncation errors
- Overflow errors
- Underflow errors
- Modeling errors
- Ill-conditioning errors

24

Consequences of errors

- **[The Patriot Missile Failure]**
- [ESA: Ariane 5 Launcher]

Example: Remedy to errors

Example Problem 1.9. Write stable code to find the roots of the equation $x^2 + bx + c = 0$.
Solution: The usual quadratic formula is

$$x_{\pm} = \frac{-b \pm \sqrt{b^2 - 4c}}{2}$$

Supposing that $b \gg c > 0$, the expression in the square root might be rounded to b^2, giving two roots $x_+ = 0$, $x_- = -b$. The latter root is nearly correct, while the former has no correct digits.

To correct this problem, multiply the numerator and denominator of x_+ by $-b - \sqrt{b^2 - 4c}$ to get

$$x_+ = \frac{2c}{-b - \sqrt{b^2 - 4c}}$$

Now if $b \gg c > 0$, this expression gives root $x_+ = -c/b$, which is nearly correct. This leads to the pair:

$$x_- = \frac{-b - \sqrt{b^2 - 4c}}{2}, \quad x_+ = \frac{2c}{-b - \sqrt{b^2 - 4c}}$$

Note that the two roots are nearly reciprocals, and if x_- is computed, x_+ can easily be computed with little additional work.

Measures of errors (precision)

- Regarding to a number
  - Absolute error
  - Relative error
- Regarding to a function
  - L_infty norm
  - L_1 norm
  - L_2 norm

Matlab Basics

- Format short, long, short e,
- String, print (fprintf)
- Arithemetic operations
- Mathematical functions
- Vectors (column, row)
- Colon, semi-colon
- Linspace, logspace
- Array arithmetic
- String functions

See appendix A 1-11

Summary

- Necessarity of having basic NM
- Number representation and errors
  - Floating-point representation
- Start with Matlab

- Next lecture – series approximation of functions