

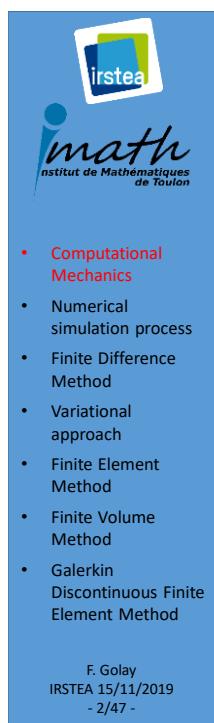
Computational Mechanics

GOLAY Frédéric

Institut de Mathématique de Toulon (IMATH)
Responsable du parcours «Modélisation et Calculs Fluides-Structures» (MOCA),
de l'école d'ingénieur de l'université de Toulon (SEATECH)

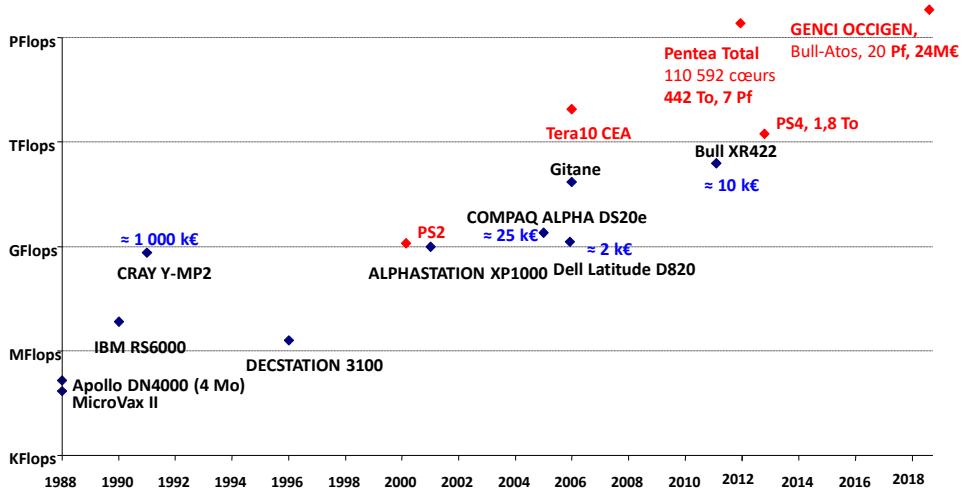
frederic.golay@univ-tln.fr

<http://freddy.univ-tln.fr>



Computational Mechanics

Evolution of computers



irstea
institut de Mathématiques
de Toulon

imath

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEAD 15/11/2019
- 3/47 -

Computational Mechanics

Evolution of computational mechanics

Aim:

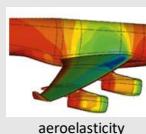
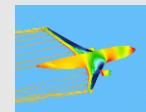
- Reproduce to explain the inaccessible
- Plan before you realize

Replace
Theory-Experiment
by

Theory-computation-Experiment

Evolution:

- Multiphysics
- Multiscale
- High Performance Computing



Sources : engineering.swan
ONERA & Lecture NF04 UTC



Conception

Simulation

Experiment

Production

irstea
institut de Mathématiques
de Toulon

imath

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEAD 15/11/2019
- 4/47 -

Computational Mechanics

Continuum mechanics

Conservation of mass

$$\frac{dp}{dt} + \rho \operatorname{div} \vec{v} = 0$$

or $\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \vec{v}) = 0$

Balance of linear momentum

$$\begin{cases} \operatorname{div} \vec{\sigma} + \vec{f} = \rho \vec{\gamma} & \text{dans } \Omega \\ \vec{\sigma} \vec{n} = \vec{F} & \text{sur } \partial \Omega \end{cases}$$

Balance of angular momentum

$$\vec{\sigma} = \vec{\sigma}^T$$

Conservation of energy

$$\frac{de}{dt} = \vec{\sigma} : \vec{D} = \vec{r} \cdot \operatorname{div} \vec{v}$$

[m] \vec{x} : actual position

[s] t : time

(\vec{x}, t) : Eulerian variables

Material derivative

$$\frac{d}{dt} = \frac{\partial}{\partial t} + (\vec{v} \cdot \nabla)$$

[kg/m³] $\rho(\vec{x}, t)$: density

[m/s] $\vec{v}(\vec{x}, t)$: velocity

[N/m³] \vec{f} : body force per unit volume acting in Ω

[N/m²] \vec{F} : contact force per unit surface acting on $\partial \Omega$

[–] \vec{n} : outward normal vector of $\partial \Omega$

[m/s²] $\vec{\gamma}$: acceleration

$$\vec{\gamma}(\vec{x}, t) = \frac{d\vec{v}}{dt} = \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v}$$

[N/m²] $\vec{\sigma}(\vec{x}, t)$: Second order Cauchy stress tensor

[W/kg] e : specific internal energy

$$[\text{s}^{-1}] \vec{D} : \text{strain-rate (or stretching) tensor} \quad \vec{D} = \frac{1}{2} (\nabla^T \vec{v} + \nabla \vec{v})$$

[W/m²] \vec{q} : heat flux

[W/m³] r : heat supply density

irstea
imath
Institut de Mathématiques de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 5/47 -

Computational Mechanics

Example: Wave breaking



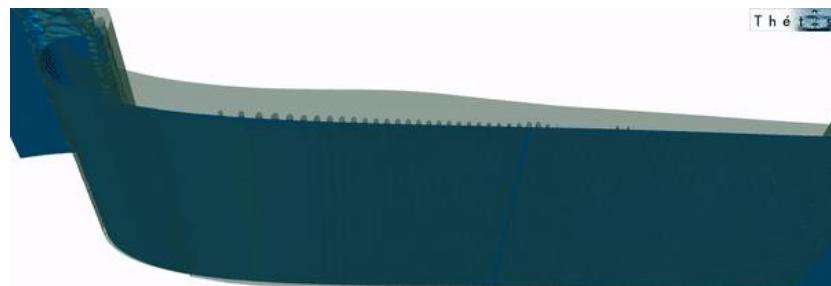
irstea
imath
Institut de Mathématiques de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 6/47 -

Computational Mechanics

Example: Wave breaking, full Navier-Stokes Air-Water simulation



P. Lubin, S. Glockner I2M Bordeaux, France, software Thétis

80 Millions cells on 1024 cores

800 Millions cells on 4096 cores

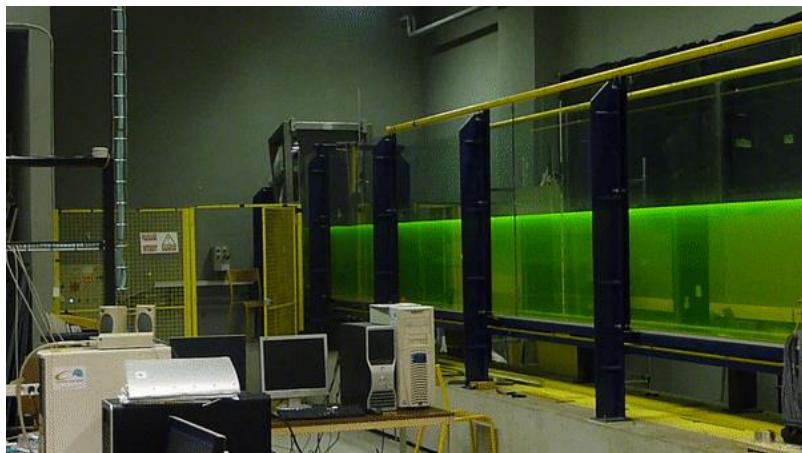
irstea
imath
*Institut de Mathématiques
de Toulon*

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 7/47 -

Computational Mechanics

Example: Wave propagation, wave breaking experiment



Olivier Kimmoun, ECM, Marseille France, workshop B'Waves 2014 Bordeaux

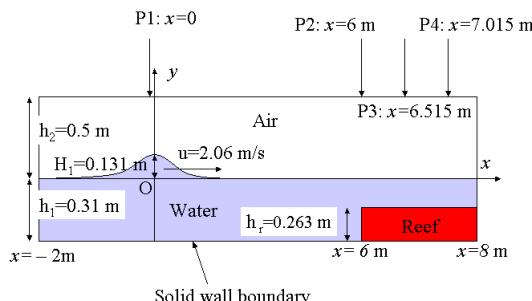
irstea
imath
*Institut de Mathématiques
de Toulon*

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 8/47 -

Computational Mechanics

Example: : Wave propagation, wave breaking experiment



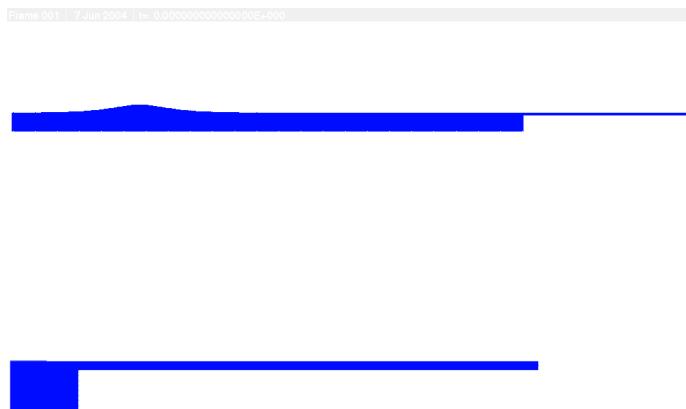
irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 9/47 -

Computational Mechanics

Example: Wave propagation, wave breaking Air-Water Euler model (Finite Volume)



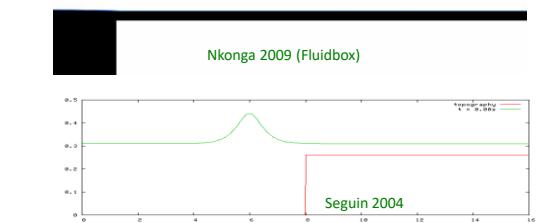
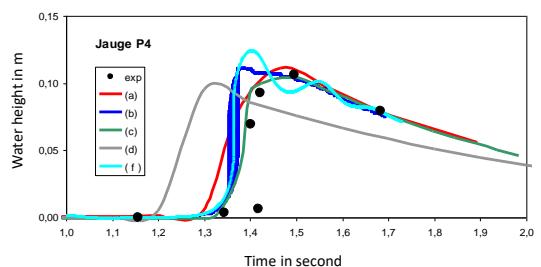
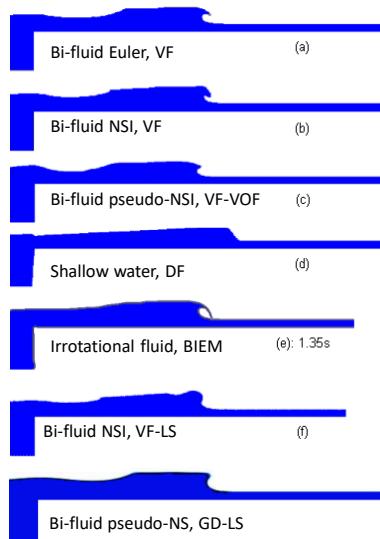
irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 10/47 -

Computational Mechanics

Confrontation of several CFD codes



P. Helluy, F. Golay, J.-P. Caltagirone, P. Lubin, S. Vincent, D. Drevard, R. Marcer, P. Fraunie, N. Seguin, S. Grilli, A.N. Lesage, A. Dervieux, O. Allain, "Numerical simulation of wave breaking", M2AN, Vol.39 n°3, pp 591-607, 2005

B. Braconnier, J-J Hu, Y-Y Niu, B. Nkonga, K-M Shyue , Numerical simulations of low Mach compressible two-phase flows: Preliminary assessment of some basic solution techniques, ESAIM: Proc., Vol. 28, pp. 117-134, 2009.

irstea

imath
Institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 11/47 -

Computational Mechanics

Example, metal forming using finite elements (Forge3D – Cemef)



irstea

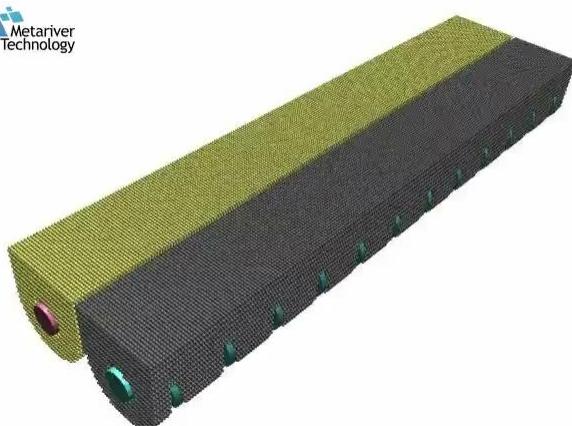
imath
Institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 12/47 -

Computational Mechanics

Example of computation on GPU (DEM+Cuda)



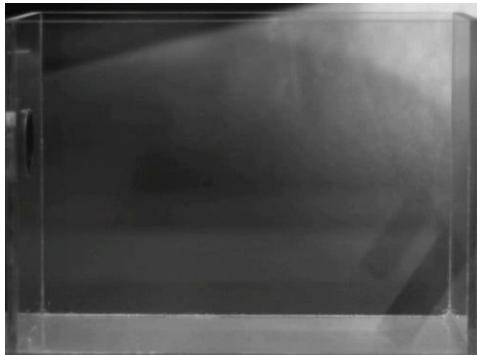
irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

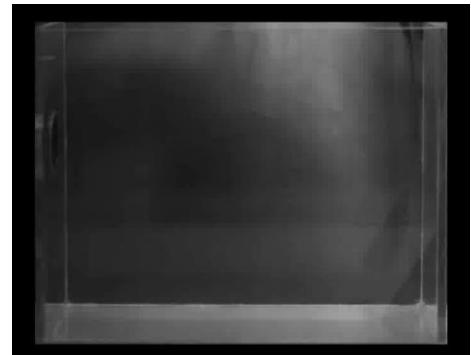
F. Golay
IRSTEA 15/11/2019
- 13/47 -

Computational Mechanics

Realistic image rendering example applied to fluid mechanics



Experiment



Numerical simulation:
FEM/VMS + LES +
Convected Level Set...
+ blender

Elie Hachem, Thierry Coupez, Cemef, code CimLib, anisotropic adaptive mesh refinement technic

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 14/47 -

Computational Mechanics

Overview of numerical **approximation** of partial differential equations

- Finite Difference Method (FDM)
- Finite Element Method (FEM)
- Finite Volume Method (FVM)
- Spectral Method
- Boundary Element Method (BEM)
- Lattice Boltzmann (LB)
- Smooth Particle Hydrodynamics (SPH)
- Discrete Element Method (DEM)
- Many others ...

Finite Difference Method (FDM)

The oldest method, used for many physics

- Easy to implement
- Easy to make higher order
- Only applicable on structured grids
- Does not fit the geometry

Finite Element Method (FEM)

Usually used in structure mechanics

- Any order of accuracy
- Based on variational methods
- Applicable on unstructured/complex grids
- Naturally implicit, well-adapted to non-linear behaviour
- Excellent for diffusion dominated problem
- Naturally implicit, need sparse linear solver (can be expensive for large systems)
- Not conservative
- More complex

Finite Volume Method (FVM)

Usually used in fluid mechanics

- Applicable on unstructured/complex grids
- Naturally conservative, capture discontinuities
- Easy explicit formulation (parallel computation)
- Difficult to devise stable higher order scheme
- Not very accurate for diffusion dominated problem
- More complex

irstea
math
*institut de Mathématiques
de Toulon*

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 15/47 -

Numerical simulation process

What does computing engineer mean?



system analysis, determination of the main phenomena, ...
Fluid flows, wave propagation, wave breaking, impact, fluid-structure interaction, structural analysis, ...

irstea
math
*institut de Mathématiques
de Toulon*

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 16/47 -

Numerical simulation process

What does computing engineer mean?

System analysis, modelization ,... Fluid flow



Mechanical / Mathematical Modelization

Model 1: Shallow water

$$\begin{cases} \frac{\partial h}{\partial t} + \operatorname{div}(h\vec{u}) = 0 \\ \frac{\partial h\vec{u}}{\partial t} + \operatorname{div}(h\vec{u} \otimes \vec{u} + g \frac{h^2}{2}) = -\rho h \nabla Z + \dots \end{cases}$$

?

Model 2: Navier Stokes

$$\begin{cases} \operatorname{div}(\vec{v}) = 0 \\ \frac{\partial \vec{v}}{\partial t} + \nabla \cdot \vec{v} \cdot \vec{v} = -\frac{1}{\rho} \nabla p + \nu \Delta \vec{v} \end{cases}$$

Model 4:

Model 3: Euler two-phase

$$\begin{cases} \frac{\partial \rho \vec{u}}{\partial t} + \operatorname{div}(\rho \vec{u} \otimes \vec{u} + \bar{\rho} \vec{g}) = \rho \bar{g} \\ \frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho = 0 \end{cases}$$

irstea
math
Institut de Mathématiques de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 17/47 -

Numerical simulation process

What does computing engineer mean?

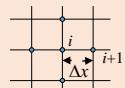
System analysis, modelization ,... Fluid Flow



Mechanical / Mathematical Modelization : Bifluid Euler

Numerical formulation, discrete approach

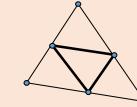
Model 1: FDM



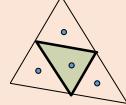
?

Model 4: SPH

Model 2: FEM



Model 3: FVM



Numerical simulation process

What does computing engineer mean?

System analysis, modelization ,... -> Fluid flow



Mechanical / Mathematical Modelization -> Bifluid Euler

Numerical formulation, discrete approach -> FVM

Numerical method, solver

Spatial discretisation: order, gradient, ...

Time discretization: explicit, implicit, ...

Solver: direct, iterative, ...

Domain decompositon, mesh refinement, ...

Numerical improvement, ...

irstea
math
Institut de Mathématiques de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 18/47 -

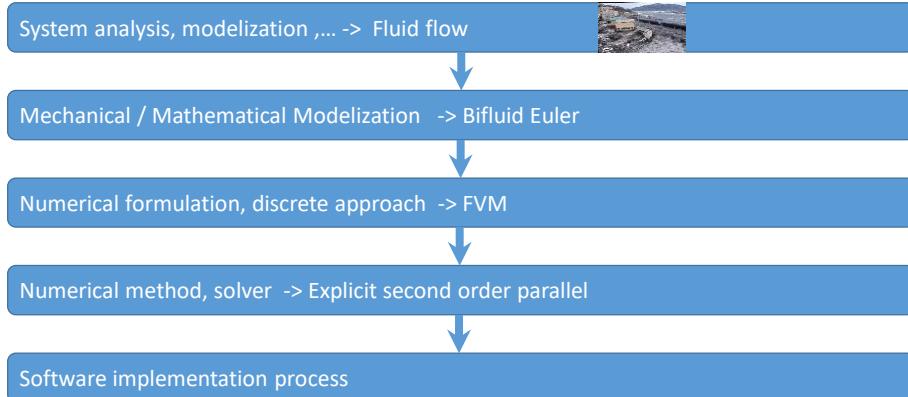
irstea
math
*institut de Mathématiques
de Toulon*

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 19/47 -

Numerical simulation process

What does computing engineer mean?



Programmation: C, fortran90, C++, ...

Parallel: Cuda, MPI, ...

Computer-aided software engineering, Scientific programming, versioning, ...

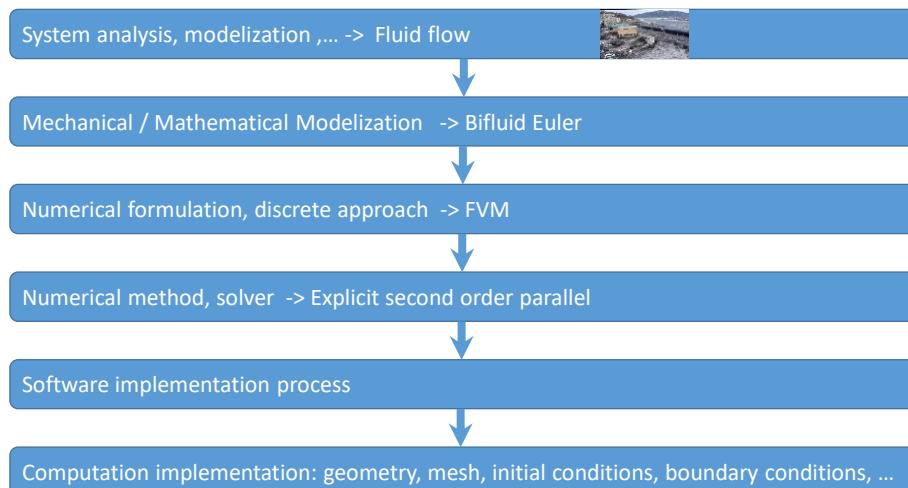
irstea
math
*institut de Mathématiques
de Toulon*

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 20/47 -

Numerical simulation process

What does computing engineer mean?



Preprocessing: can be very time-consuming

irstea
i-math
*institut de Mathématiques
de Toulon*

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 21/47 -

Numerical simulation process

What does computing engineer mean?

System analysis, modelization ,... -> Fluid flow 

Mechanical / Mathematical Modelization -> Bifluid Euler

Numerical formulation, discrete approach -> FVM

Numerical method, solver -> Explicit second order parallel

Software implementation process

Computation implementation: geometry, mesh, initial conditions, boundary conditions, ...

Run !

HPC: High Performance Computing

irstea
i-math
*institut de Mathématiques
de Toulon*

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 22/47 -

System analysis, modelization ,... -> Fluid flow 

Mechanical / Mathematical Modelization -> Bifluid Euler

Numerical formulation, discrete approach -> FVM

Numerical method, solver -> Explicit second order parallel

Software implementation process

Computation implementation: geometry, mesh, initial conditions, boundary conditions, ...

Run !

Very critical analysis of the results

irstea
i-math
Institut de Mathématiques de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 23/47 -

Numerical simulation process

What does computing engineer mean?

Frame 001 | 7-Jun-2004 | t= 0.00000000000000E+000



CFD = Computational Fluid Dynamics

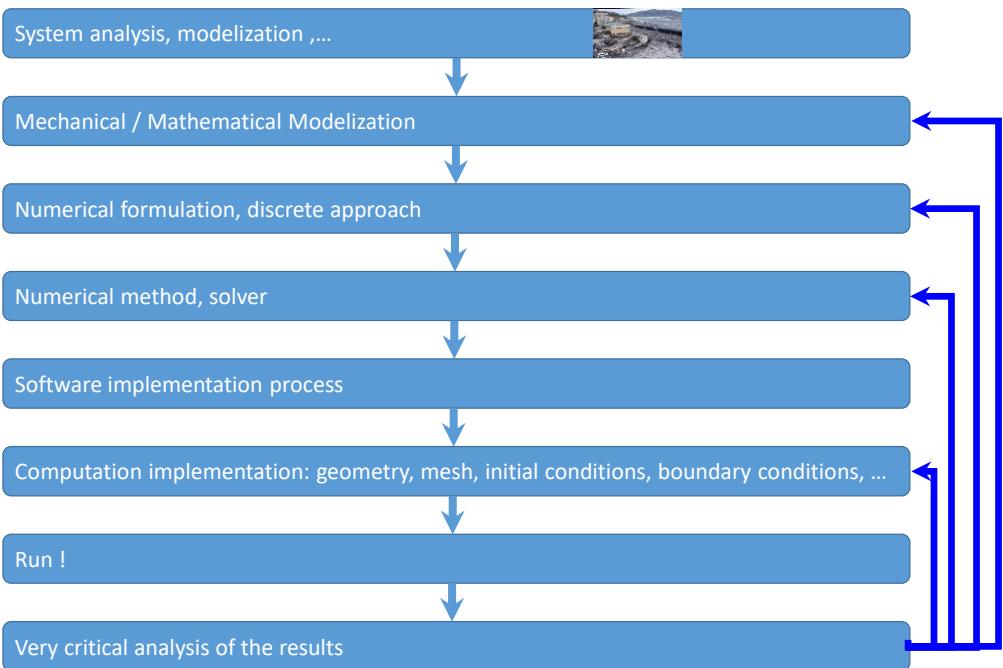
CFD ≠ Color Fluid Dynamics (G. Allaire ?)



irstea
i-math
Institut de Mathématiques de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 24/47 -



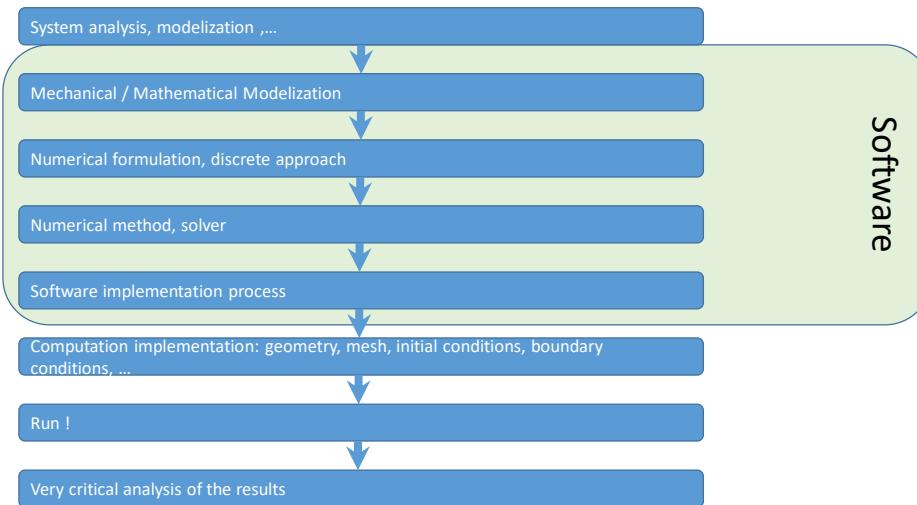
irstea
institut de Mathématiques de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 25/47-

Numerical simulation process

What does computing engineer mean?



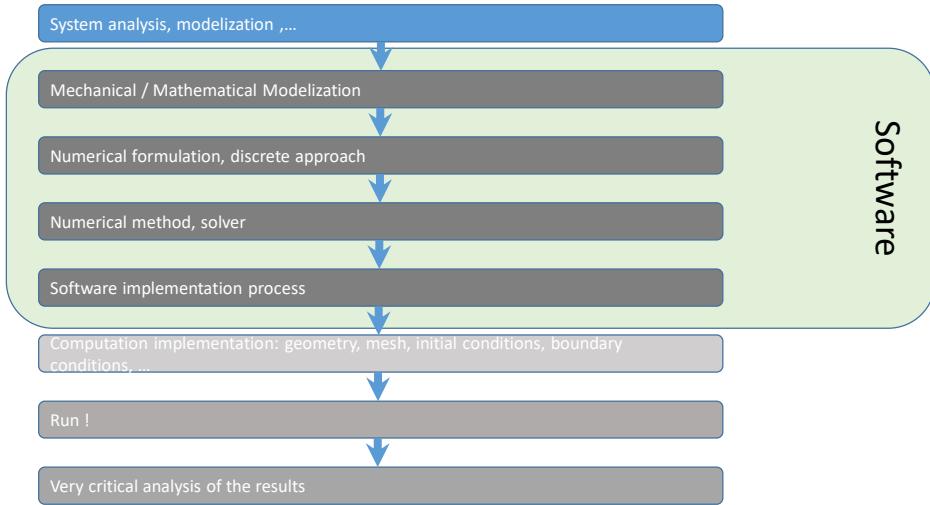
irstea
institut de Mathématiques de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 26/47 -

Numerical simulation process

What does computing engineer mean?



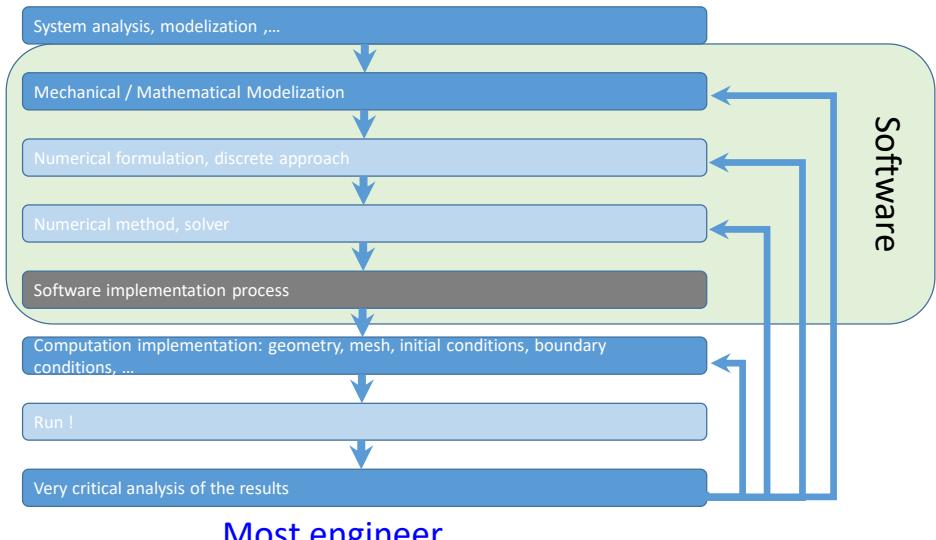
irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 27/47 -

Numerical simulation process

What does computing engineer mean?



Most engineer

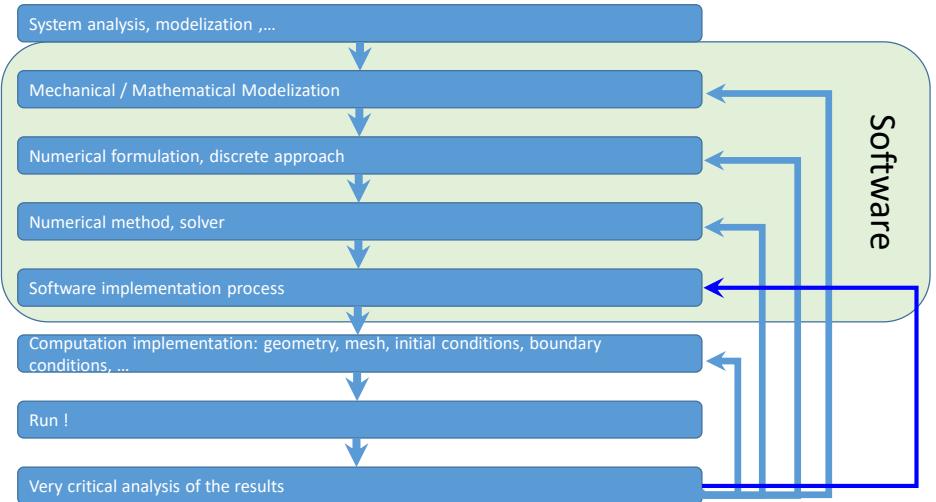
irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 28/47 -

Numerical simulation process

What does computing engineer mean?



Engineer in computational Mechanics



imath
Institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 29/47 -

Finite Difference Method

Taylor's Theorem

Let u be an n -times differentiable function on an open interval containing the points $x+h$ and x , then :

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2!}u''(x) + \frac{h^3}{3!}u'''(x) + \dots + \frac{h^{n-1}}{(n-1)!}u^{(n-1)}(x) + O(h^n)$$

Where $O(h^n) = \frac{h^n}{n!}u^n(c)$ and c is between x and $x+h$

Finite difference approximation of the first derivative of u

Forward first order finite difference approximation of u'

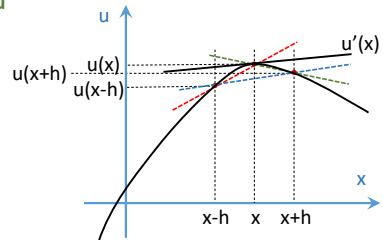
$$u(x+h) = u(x) + hu'(x) + O(h^2) \quad u'(x) = \frac{u(x+h) - u(x)}{h} + O(h)$$

Backward first order finite difference approximation of u'

$$u(x-h) = u(x) - hu'(x) + O(h^2) \quad u'(x) = \frac{u(x) - u(x-h)}{h} + O(h)$$

Centered first order finite difference approximation of u'

$$u'(x) = \frac{u(x+h) - u(x-h)}{2h} + O(h)$$




imath
Institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 30/47 -

Finite Difference Method

Finite difference approximation of the second derivative of u

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(x) + O(h^4)$$

$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u'''(x) + O(h^4)$$

$$u(x+h) + u(x-h) = 2u(x) + h^2u''(x) + O(h^4)$$

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} + O(h^2)$$

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

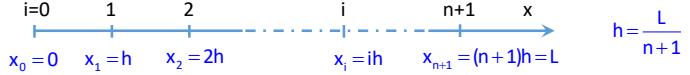
F. Golay
IRSTEA 15/11/2019
- 31/47 -

Finite Difference Method Elliptic equation

1D discretization of the Laplacian operator

$$\Delta u = 0$$

$$\frac{\partial^2 u}{\partial x^2} = 0$$



$$\text{Notation } u(x_i) = u_i$$

$$\forall i=1,n \quad u''(x_i) \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = 0$$

Finite Difference Method Elliptic equation

2D discretization of the Laplacian operator

$$u(x+h_x, y+h_y) = \sum_{0 \leq j+k \leq p} \frac{h_x^j h_y^k}{j! k!} \frac{\partial^{j+k} u(x, y)}{\partial x^j \partial y^k}$$

$$\Delta u(x, y) = 0$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

$$u(x+h_x, y) = u(x, y) + h_x \frac{\partial u(x, y)}{\partial x} + \frac{h_x^2}{2} \frac{\partial^2 u(x, y)}{\partial x^2} + \frac{h_x^3}{6} \frac{\partial^3 u(x, y)}{\partial x^3} + O(h_x^4)$$

$$u(x-h_x, y) = u(x, y) - h_x \frac{\partial u(x, y)}{\partial x} + \frac{h_x^2}{2} \frac{\partial^2 u(x, y)}{\partial x^2} - \frac{h_x^3}{6} \frac{\partial^3 u(x, y)}{\partial x^3} + O(h_x^4)$$

$$u(x, y+h_y) = u(x, y) + h_y \frac{\partial u(x, y)}{\partial y} + \frac{h_y^2}{2} \frac{\partial^2 u(x, y)}{\partial y^2} + \frac{h_y^3}{6} \frac{\partial^3 u(x, y)}{\partial y^3} + O(h_y^4)$$

$$u(x, y-h_y) = u(x, y) - h_y \frac{\partial u(x, y)}{\partial y} + \frac{h_y^2}{2} \frac{\partial^2 u(x, y)}{\partial y^2} - \frac{h_y^3}{6} \frac{\partial^3 u(x, y)}{\partial y^3} + O(h_y^4)$$

$$\frac{\partial^2 u(x, y)}{\partial x^2} + \frac{\partial^2 u(x, y)}{\partial y^2} = \frac{u(x+h_x, y) - 2u(x, y) + u(x-h_x, y)}{h_x^2} + \frac{u(x, y+h_y) - 2u(x, y) + u(x, y-h_y)}{h_y^2} + O(h_x^2) + O(h_y^2)$$

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 32/47 -

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 33/47 -

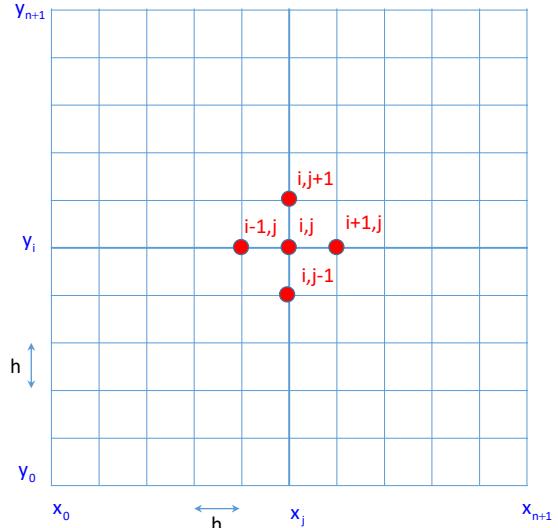
Finite Difference Method Elliptic equation

2D five points stencil

Notation $u(x_i, y_j) = u_{i,j}$

$$\forall i, j = 1, n$$

$$\Delta u(x_i, y_j) \approx \frac{u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1}}{h^2} = 0$$



irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 34/47 -

Finite Difference Method Parabolic equation

1D discretization

$$\begin{cases} \frac{\partial u}{\partial t}(x, t) - \lambda \Delta u = 0 \\ u(x, 0) = u_0(x) \end{cases}$$



Notation $u(x_i, t_n) = u_i^n$

$$\frac{\partial u}{\partial t}(x_i, t_n) \approx \frac{u_i^{n+1} - u_i^n}{\delta t} \quad \text{First order approximation}$$

Time discretisation: explicit Euler scheme

$$\frac{u_i^{n+1} - u_i^n}{\delta t} = \lambda \frac{\partial^2 u}{\partial x^2}(x_i, t_n) \approx \lambda \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2} \rightarrow u_i^{n+1} = u_i^n + \frac{\lambda \delta t}{h^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

Time discretisation: implicit Euler scheme

$$\frac{u_i^{n+1} - u_i^n}{\delta t} = \lambda \frac{\partial^2 u}{\partial x^2}(x_i, t_{n+1}) \approx \lambda \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{h^2} \rightarrow -u_i^{n+1} + \left(\frac{h^2}{\lambda \delta t} + 2 \right) u_i^{n+1} - u_{i-1}^{n+1} = \frac{h^2}{\lambda \delta t} u_i^n$$

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method**
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 35/47 -

Finite Difference Method Parabolic equation

Time discretisation: semi-implicit scheme

$$\frac{u_i^{n+1} - u_i^n}{\delta t} = \theta \lambda \frac{\partial^2 u}{\partial x^2}(x_i, t_{n+1}) + (1-\theta) \frac{\partial^2 u}{\partial x^2}(x_i, t_n) \approx \theta \lambda \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{h^2} + (1-\theta) \lambda \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2}$$

$$A = \begin{bmatrix} 2 & -1 & 0 & \cdots & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & & & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \ddots & -1 & 2 & -1 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & 0 & -1 & 2 & -1 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 2 \end{bmatrix} \quad U^n = \begin{pmatrix} u_1^n \\ \vdots \\ u_M^n \end{pmatrix} \quad \left(I_d + \frac{\theta \lambda \delta t}{h^2} A \right) U^{n+1} = \left(I_d - \frac{(1-\theta) \lambda \delta t}{h^2} A \right) U^n$$

$\theta=0$ explicit scheme: Forward Euler

Conditionally stable

$\theta=1$ implicit scheme: Backward Euler

Unconditionally stable

$\theta=0,5$ semi implicit scheme: Crank-Nicholson

Unconditionally stable for $\theta \geq 0,5$

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Variational approach**
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 36/47 -

Variational approach

Principle

$$\frac{d\vec{w}}{dt} + \text{div}\vec{F}(\vec{w}) = \vec{S} \quad \text{in } \Omega$$

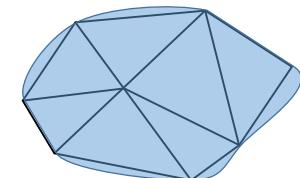
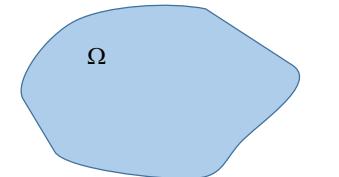
$$\int_{\Omega} \vec{\varphi} \cdot \left(\frac{d\vec{w}}{dt} + \text{div}\vec{F} \right) dv = \int_{\Omega} \vec{\varphi} \cdot \vec{S} dv \quad \forall \vec{\varphi} \dots$$

The computational domain Ω is split in several cells or elements

$$\int_{\Omega} \dots dv = \sum_e \int_{\Omega_e} \dots dv$$

$$\sum_e \int_{\Omega_e} \vec{\varphi} \cdot \frac{d\vec{w}}{dt} dv + \sum_e \int_{\Omega_e} \vec{\varphi} \cdot \text{div}\vec{F} dv = \sum_e \int_{\Omega_e} \vec{\varphi} \cdot \vec{S} dv$$

$$\sum_e \int_{\Omega_e} \vec{\varphi} \cdot \frac{d\vec{w}}{dt} dv - \sum_e \int_{\Omega_e} \nabla \vec{\varphi} : \vec{F}^T dv + \sum_e \int_{\Omega_e} \text{div}(\vec{F}^T \vec{\varphi}) dv = \sum_e \int_{\Omega_e} \vec{\varphi} \cdot \vec{S} dv$$



$$\text{div}(\vec{F}^T \vec{\varphi}) = \nabla \vec{\varphi} : \vec{F}^T + \vec{\varphi} \cdot \text{div}\vec{F}$$

Green's formula

$$\sum_e \int_{\Omega_e} \vec{\varphi} \cdot \frac{d\vec{w}}{dt} dv - \sum_e \int_{\Omega_e} \nabla \vec{\varphi} : \vec{F}^T dv + \sum_e \int_{\partial\Omega_e} \vec{\varphi} \cdot \vec{F}^T \vec{n} ds = \sum_e \int_{\Omega_e} \vec{\varphi} \cdot \vec{S} dv$$

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- **Finite Element Method**
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 37/47 -

Finite Element Method

Principle

$$\frac{d\vec{w}}{dt} + \operatorname{div}\vec{F}(w) = \vec{S} \quad \text{in } \Omega$$

$$\sum_e \int_{\Omega_e} \vec{\varphi} \cdot \frac{d\vec{w}}{dt} \, dv - \sum_e \int_{\Omega_e} \nabla \vec{\varphi} : \vec{F}^T \, dv + \sum_e \int_{\partial\Omega_e} \vec{\varphi} \cdot \vec{F}_n \, ds = \sum_e \int_{\Omega_e} \vec{\varphi} \cdot \vec{S} \, dv$$

The solutions w are approximated in each Element by a polynomial approximation

$$\vec{w}_e(x, y, z) \approx \sum_{\text{nodes of } e} N_i(x, y, z) \vec{w}_i$$

Where N_i are chosen polynomials of order 1, 2, 3, ... called interpolation functions

Rmk 1: $N_i = 1$ on node i and : $N_i = 0$ on other nodes

Rmk 2: the approximation of w is continuous!

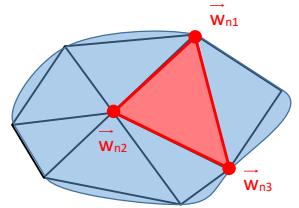
Rmk 3: the approximation of ∇w is NOT continuous!

$$\vec{\varphi} \text{ is chosen as a continuous test function} \Rightarrow \sum_e \int_{\partial\Omega_e} \vec{\varphi} \cdot \vec{F}_n \, ds = \sum_e \int_{\partial\Omega_e} \vec{\varphi} \cdot \vec{F}_n \, ds \quad \text{Neumann condition}$$

$$\text{Using the Galerkin's rule the test functions are chosen such that: } \vec{\varphi}(x, y, z) \approx \sum_{\text{nodes of } e} N_i(x, y, z) \vec{\varphi}_i$$

$$\sum_e \int_{\Omega_e} N_j \vec{\varphi}_j \cdot \frac{d}{dt} N_i \vec{w}_i \, dv - \sum_e \int_{\Omega_e} \nabla N_j \vec{\varphi}_j : F(N_i \vec{w}_i) \, dv = \sum_e \int_{\Omega_e} N_j \vec{\varphi}_j \cdot \vec{S} \, dv - \sum_e \int_{\partial\Omega_e} N_j \vec{\varphi}_j \cdot \vec{F}_n \, ds \quad \forall \vec{\varphi}_j$$

therefore taking successively each component of the test functions equal to 1 and the others to zero, we obtain a system of equations of size : number of degree of freedom x number of nodes



irstea
institut de Mathématiques
de Toulon

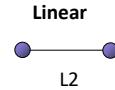
- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- **Finite Element Method**
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 38/47 -

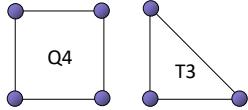
Finite Element Method

Some usual finite element types

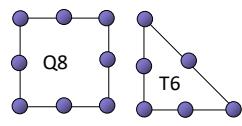
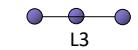
1D



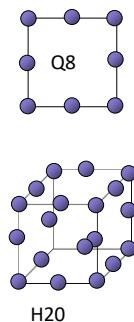
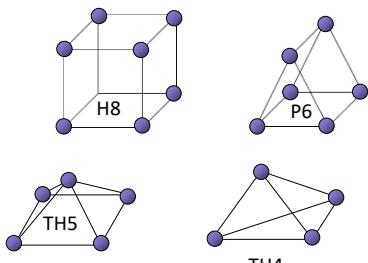
2D



Quadratic



3D



irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- **Finite Element Method**
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 39/47 -

Finite Element Method

Reference Element

$$\bar{x}(x, y, z) \approx \sum_{\text{nodes of } e} \bar{N}_i(x, y, z) \bar{x}_i \quad \bar{N}_i \text{ denote the shape functions}$$

In the case of isoparametric element, we get $\bar{N}_i = N_i$

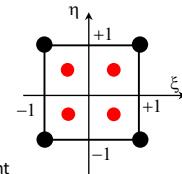
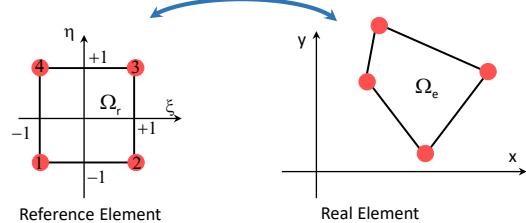
$$\int_{\Omega_e} \dots dx dy = \int_{\Omega_r} \dots \det J d\xi d\eta$$

Where J denotes the Jacobian of the transformation

Numerical integration

$$\int_{\Omega_r} f(\xi, \eta) d\xi d\eta = \sum_{\text{Gauss points}} \omega_{PG} f(\xi_{PG}, \eta_{PG})$$

According to the Gaussian quadrature rule, ω_{PG} denotes the weights of each Gaussian point



irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- **Finite Element Method**
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 40/47 -

Finite Element Method

Many other notions specific to FEM to handle ...

- Mesh
- Conforming mesh
- Assembly
- Lumping
- Post processing analysis
- ...



Many other notions to handle in the framework of FEM

- Boundaries conditions
- Time discretisation
- Linear solver: direct, iterative
- Non-linearities, tangent operator
- Convergence
- A posteriori error
- Domain decomposition
- Adaptive mesh refinement
- HPC
- ...

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 41/47 -

Finite Volume Method

Principle

$$\frac{d\bar{w}}{dt} + \operatorname{div}\bar{F}(w) = \bar{S} \quad \text{in } \Omega$$

$$\sum_e \int_{\Omega_e} \bar{\varphi} \cdot \frac{d\bar{w}}{dt} \, dv - \sum_e \int_{\partial\Omega_e} \nabla \bar{\varphi} : \bar{F}^T \, ds + \sum_e \int_{\partial\Omega_e} \bar{\varphi} \bar{F} \cdot \bar{n} \, ds = \sum_e \int_{\Omega_e} \bar{\varphi} \bar{S} \, dv$$

The solutions w are approximated in each volume by an average value

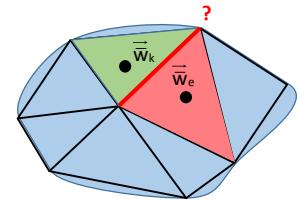
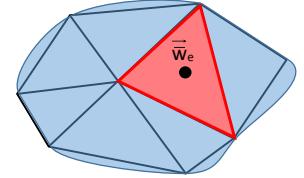
$$\bar{w}_e(x, y, z) \approx \frac{1}{|\Omega_e|} \int_{\Omega_e} \bar{w} \, dv$$

$\bar{\varphi}$ is chosen successively as **constant** on volume Ω_e and null elsewhere

$$\Rightarrow \nabla \bar{\varphi} = \bar{0}$$

$$\Rightarrow \int_{\Omega_e} \frac{d\bar{w}}{dt} \, dv + \int_{\partial\Omega_e} \bar{F} \cdot \bar{n} \, ds = \int_{\Omega_e} \bar{S} \, dv$$

$$\Rightarrow \frac{d\bar{w}_e}{dt} + \int_{\partial\Omega_e} \bar{F}(\bar{w}_e) \cdot \bar{n} \, ds = \bar{S} \quad \bar{F}(\bar{w}_e) \text{ is NOT defined on } \partial\Omega_e!$$

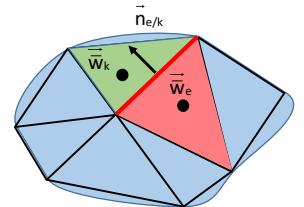


Finite Volume Method

Fluxes computation

$$\int_{\partial\Omega_e} \bar{F} \cdot \bar{n} \, ds \approx \sum_{\text{edges}} |\text{edge}| f(\bar{w}_e, \bar{w}_k, \bar{n}_{e/k})$$

- Centered
- Roe
- Lax-Friedrichs
- Engquist-Osher
- Lax-Wendroff
- Godunov : exact Riemann solver
- ...



irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 42/47 -

irstea
institut de Mathématiques
de Toulon

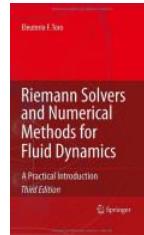
- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method**
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 43/47 -

Finite Volume Method

Many other notions specific to FVM to handle ...

- Structured Mesh, unstructured mesh
- Second order reconstruction (MUSCL)
- Slope limiters
- Post processing analysis
- ...



Many other notions to handle in the framework of FVM

- Boundaries conditions
- Time discretisation
- Linear solver: direct, iterative, multigrid
- Interface sharpening
- Numerical diffusion
- Convergence
- A posteriori error
- Domain decomposition, parallel computing
- Adaptive mesh refinement
- HPC
- ...

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method**
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 44/47 -

Galerkin Discontinuous Finite Element Method

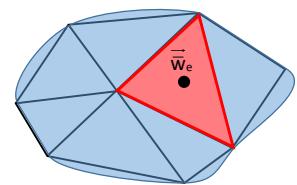
Principle

$$\frac{d\vec{w}}{dt} + \operatorname{div}\vec{F}(w) = \vec{S} \quad \text{in } \Omega$$

$$\sum_e \int_{\Omega_e} \vec{\varphi} \cdot \frac{d\vec{w}}{dt} \, dv - \sum_e \int_{\Omega_e} \nabla \vec{\varphi} : \vec{F}^T \, dv + \sum_e \int_{\partial\Omega_e} \vec{\varphi} \cdot \vec{F}_n \, ds = \sum_e \int_{\Omega_e} \vec{\varphi} \cdot \vec{S} \, dv$$

The solutions w are approximated in each Element by a polynomial approximation of order p

$$\vec{w}_e(x, y, z) \approx \sum_{i,j,k=0}^{i+j+k=p} a_{ijk} x^i y^j z^k$$



Rmk 1: the approximation of w NOT is continuous!

Rmk 2: We present a monomial approach, easier to implement, but harder to physically understand. A nodal approximation is still possible

$\vec{\varphi}$ Is chosen successively as a **DIScontinuous** test function on element Ω_e and null elsewhere

Using the **Galerkin's** rule the test functions are also chosen such that: $\vec{\varphi}_e(x, y, z) \approx \sum_{i,j,k=0}^{i+j+k=p} \varphi_{ijk} x^i y^j z^k$

$$\int_{\Omega_e} \vec{\varphi}_e \cdot \frac{d\vec{w}_e}{dt} \, dv - \int_{\Omega_e} \nabla \vec{\varphi}_e : \vec{F}^T \, dv + \int_{\partial\Omega_e} \vec{\varphi}_e \cdot \vec{F}_n \, ds = \int_{\Omega_e} \vec{\varphi}_e \cdot \vec{S} \, dv \quad \forall \varphi_{ijk}$$

therefore taking successively each component of the test functions equal to 1 and the others to zero, we obtain a system of equations of size : number of degree of freedom x number of coefficient of the polynomial approximation

irstea
institut de Mathématiques
de Toulon

- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 45/47 -

Galerkin Discontinuous Finite Element Method

Fluxes Computation

$$\int_{\Omega_e} \vec{\phi}_e \cdot \frac{d\vec{w}_e}{dt} dv - \int_{\Omega_e} \nabla \vec{\phi}_e : \vec{F}^T dv + \int_{\partial \Omega_e} \vec{\phi}_e \vec{n} ds = \int_{\Omega_e} \vec{\phi}_e \vec{S} dv \quad \forall \vec{\phi}_{ijk}$$

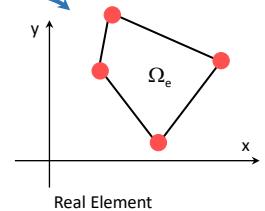
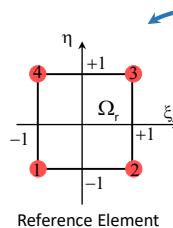
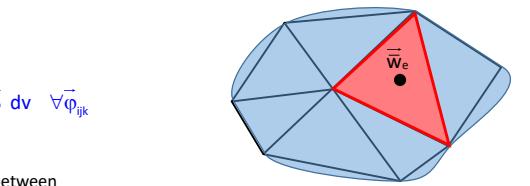
One more time, the fluxes are not defined at the interfaces between elements. An approximation has to be chosen in order to handle with the jump across the interface

Reference Element

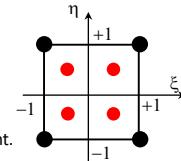
$$\vec{x}(x, y, z) \approx \sum_{\text{nodes of } e} \vec{N}_i(x, y, z) \vec{x}_i$$

$$\int_{\Omega_e} \dots dx dy = \int_{\Omega_r} \dots \det J d\xi d\eta$$

Here we use a nodal approximation, often of order 1



Reference Element



Numerical integration

$$\int_{\Omega_r} f(\xi, \eta) d\xi d\eta = \sum_{\text{Gauss points}} \omega_{PG} f(\xi_{PG}, \eta_{PG})$$

According to the Gaussian quadrature rule, ω_{PG} denotes the weights of each Gaussian point. The number of Gaussian points is adapted to the order of the polynomial approximation.

irstea
institut de Mathématiques
de Toulon

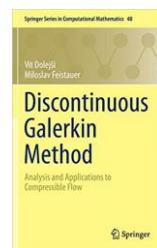
- Computational Mechanics
- Numerical simulation process
- Finite Difference Method
- Variational approach
- Finite Element Method
- Finite Volume Method
- Galerkin Discontinuous Finite Element Method

F. Golay
IRSTEA 15/11/2019
- 46/47 -

Galerkin Discontinuous Finite Element Method

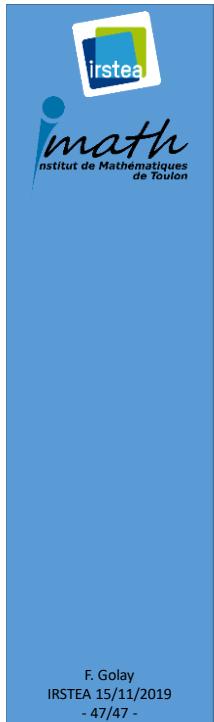
Many other notions specific to GD to handle ...

- Mesh, interface meshing
- Non conforming mesh
- Assembly
- Lumping
- Penalization
- Hp adaptation
- Post processing analysis
- ...

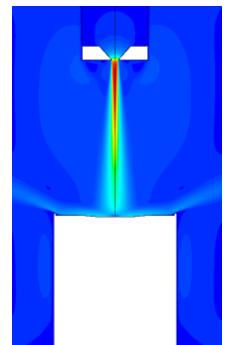
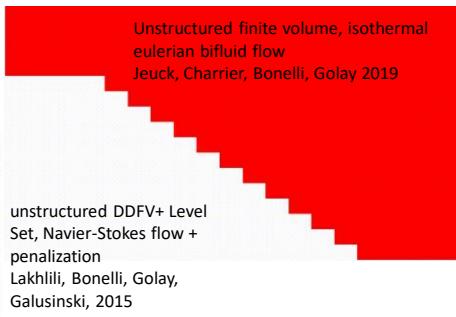
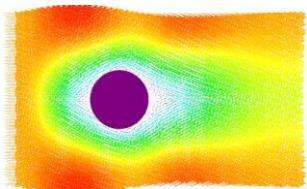


Many other notions to handle in the framework of GD

- Boundaries conditions
- Time discretisation
- Linear solver: direct, iterative
- Non-linearities, tangent operator
- Convergence
- A posteriori error
- Domain decomposition
- Adaptive mesh refinement
- HPC
- ...



To be continued



Finite volume (Fluent),
Navier-Stokes
flow+Turbulence+
remeshing
Mercier, Bonelli,
Anselmet, 2013

structured finite volume+ Level Set, MAC scheme,
Stokes flow + penalization

Lachouette, Golay, Bonelli 2009