

Discrete Mechanics

Jean-Paul Caltagirone¹

¹I2M - TREFLE - Université de Bordeaux

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Summary

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 - Continuum and Discrete Mechanics
- 2 Discrete Medium
 - Momentum equation
- 3 Thermodynamic
 - Local Thermodynamic Equilibrium hypothesis
 - Non Equilibrium Thermodynamic
- 4 Numerical methodology
 - Results on elementary cases
- 5 Applications
 - Multiphase flows

Two fundamental hypotheses

- Continuous Medium
- Local Thermodynamic Equilibrium and EOS

Differences between these two approaches

Continuum

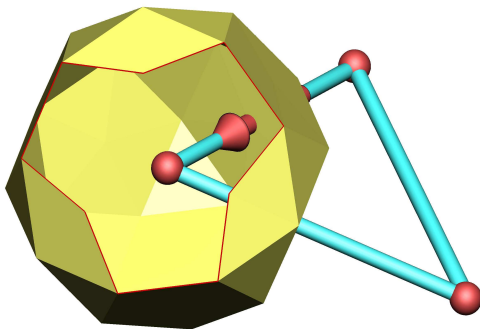
- Local Thermodynamic Equilibrium Hypothesis
- continuum : variables are defined on a point
- use of scalars, vectors, tensors
- the Lamé's coefficients are linked by Stokes's law

Discrete Medium

- L.T.E. hypothesis is discarded
- discrete approach
- use of scalars and velocity components
- compressibility and viscosity are well defined
- a decomposition of momentum equation into gradient and rotational parts

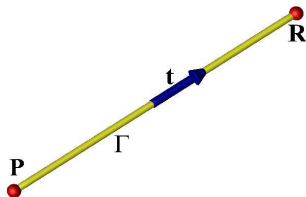
Definitions related to the topology

- discrete mechanics



- primal (blue) and dual (yellow) topologies
- velocity components and accumulation potentials (red)

Definitions of variables



- pressure, density and temperature are set to the nodes,
- the component of the velocity is constant over the edge Γ
- vorticity is defined on the faces of the primal topology,
- mean density $\bar{\rho}$ is defined as $1/L \int_P^R \rho dl$,
- the momentum $\overline{\rho \mathbf{V}}$ is constant on the edge,
- the rotational viscosity (shear) μ is constant on each face.

Discrete equation of motion

- by derivation along the unit vector \mathbf{t} we find

$$\int_{\Gamma} \rho \frac{d\mathbf{V}}{dt} \cdot \mathbf{t} dl = - \int_{\Gamma} \nabla p \cdot \mathbf{t} dl - \int_{\Gamma} \nabla_d \times (\mu \nabla_p \times \mathbf{V}) \cdot \mathbf{t} dl - \int_{\Gamma} \frac{\mu}{K} \mathbf{V} \cdot \mathbf{t} dl$$

- using the above definitions, in particular $\mu = Cte$ on each side of the primal topology, we obtain the discrete equation of motion :

$$\rho \frac{d\mathbf{V}}{dt} = -\nabla p - \nabla_d \times (\mu \nabla_p \times \mathbf{V}) - \frac{\mu}{K} \mathbf{V} + \mathbf{f}$$

Non-equilibrium flow

Non-equilibrium flow

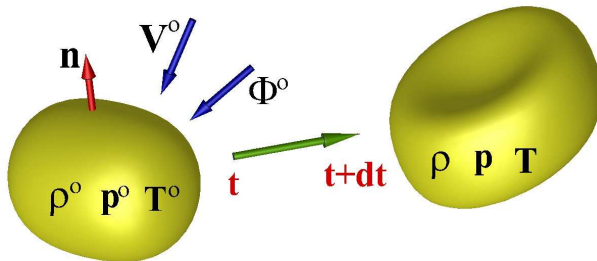
- (p, ρ, T) are not directly linked ,
- ρ is calculated by the mass conservation,
- the pressure is upgraded by the equation of motion,

Properties

- state law (ideal gaz, stiffened gas, ...) is not useful,
- the real thermodynamic coefficients are supposed known $(\beta, \chi_T, c_p, c_v)$,
- the transport properties are assumed to be know (μ, λ, k) ,
- the properties are evaluated locally by a database (NIST).

From a mechanical equilibrium to another

- \mathbf{V} and Φ are material and heat fluxes,
- p, ρ, T the pressure, density and temperature



- two equilibrium states at times t and $t + dt$

Variables

Vector variables and variable accumulation

- \mathbf{V} , the velocity and Φ , the thermal flux are vectors,
- p , pressure, ρ , density and T temperature are scalar accumulators,
- $\nabla \cdot \mathbf{V}$ and $\nabla \cdot \Phi$ to assess :
 - – ρ , density, upgraded by mass conservation,
 - – p , pressure, upgraded by momentum conservation,
 - – T , temperature, upgraded by energy conservation.

Scalar variables

- (p, ρ, T) are linked by the relation

$$\frac{d\rho}{dt} = -\frac{1}{\rho} \nabla \cdot \mathbf{V} = \left(\frac{\partial \rho}{\partial p} \right)_T \frac{dp}{dt} + \left(\frac{\partial \rho}{\partial T} \right)_p \frac{dT}{dt}$$

- by including the phase change effects (Clapeyron)

$$\frac{dp}{dt} = -\frac{1}{\chi_T} \nabla \cdot \mathbf{V} + \left(\frac{\beta}{\chi_T} + \frac{\rho_g L}{T} \right) \frac{dT}{dt}$$

- from the energy conservation we write

$$\frac{dT}{dt} = \frac{1}{\rho c_v} \nabla \cdot \Phi - \frac{\beta T}{\rho c_v \chi_T} \nabla \cdot \mathbf{V} + \frac{q}{\rho c_v} + \frac{\phi}{\rho c_v}$$

- the material derivatives are written with $\nabla \cdot \mathbf{V}$ and $\nabla \cdot \Phi$

Conservation laws and potentials

- Conservation laws for an equilibrium

$$\begin{cases} \rho \frac{d\mathbf{V}}{dt} = -\nabla p^o - \nabla \times (\mu \nabla \times \mathbf{V}) - \frac{\mu}{K} \mathbf{V} + \mathbf{f} \\ \tau \frac{d\Phi}{dt} = -\nabla T^o - \nabla \times (\nu \nabla \times \Phi) - \frac{1}{k} \Phi + \mathbf{s} \end{cases}$$

- Potentials of accumulation

$$\begin{cases} \frac{dp}{dt} = - \left(\frac{1}{\chi_T} + \frac{\beta^2 T}{\rho c_v \chi_T^2} + \frac{\rho_g L \beta}{\rho c_v \chi_T} \right) \nabla \cdot \mathbf{V} - \left(\frac{\beta}{\rho c_v \chi_T} + \frac{\rho_g L}{T \rho c_v} \right) \nabla \cdot \Phi + \dots \\ \frac{dT}{dt} = - \left(\frac{\beta T}{\rho c_v \chi_T} \right) \nabla \cdot \mathbf{V} - \left(\frac{1}{\rho c_v} \right) \nabla \cdot \Phi + \frac{q}{\rho c_v} + \frac{\phi}{\rho c_v} \\ \frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{V} \end{cases}$$

Diffusion for a linear function - different codes

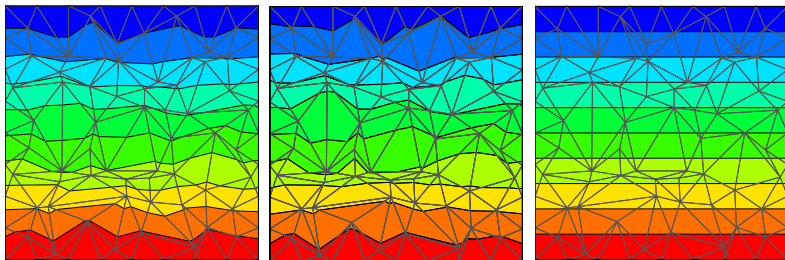


FIGURE : Stationary diffusion on unstructured mesh ; isovalues and mesh, Code A, Code B, Aquilon.

Results on elementary cases

Diffusion for a linear function

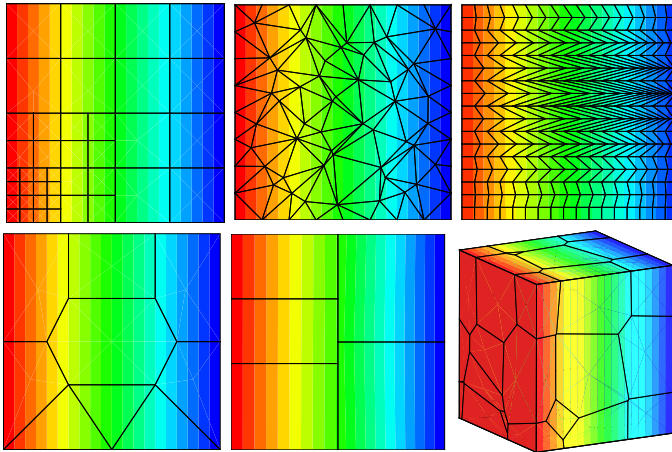


FIGURE : linear solution for different meshes.

Sloshing water-air

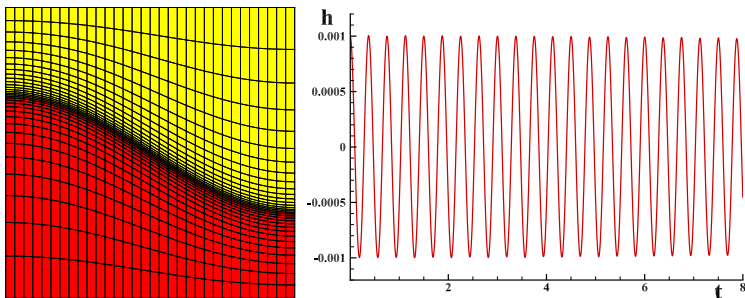


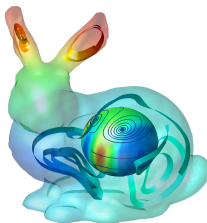
FIGURE : Sloshing at zero viscosity in small perturbations ; conservation of vorticity, liquid : $\rho = 1000$, $\mu = 0$ and gaz : $\rho = 1$, $\mu = 0$.

Conclusions

Multiphysics approach

- Continuum and LTE hypotheses are discarded
- introduce the only dual vector of the antisymmetric rotation tensor Ω
- formulation use the only the velocity components
- only one viscosity coefficient $\mu \geq 0$
- The Clausius-Duhem inequality is verified but $\Phi = \frac{dt}{\chi_T} (\nabla \cdot \mathbf{V})^2 + \mu (\nabla \times \mathbf{V})^2 \neq 0$ if $\mu = 0$,
- integrate only thermoelastic coefficients and transport properties
- introduce dt/χ_T a robust coefficient reflecting a the physics of compressible flows

END



Simulation of Marangoni currents on a surface bubble included in a bunny by Discrete Operator Calculus

- **HAL** : Jean-Paul Caltagirone : Mécanique des Milieux Discrets, <http://hal.archives-ouvertes.fr/hal-00788639>
- J-P. Caltagirone, C. Caruyer, S. Vincent, A multiphase compressible model for the simulation of multiphase flows, Computers & Fluids, vol. 50, no. 1, pp. 24-34, 2011.