Collaborative computational frameworks and the growth problem

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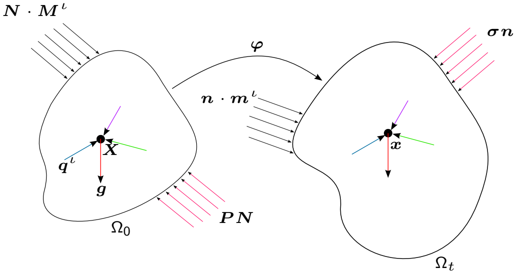
September 4th, 2008 – Oberwolfach-Walke

Returning to the model: A Lagrangian perspective

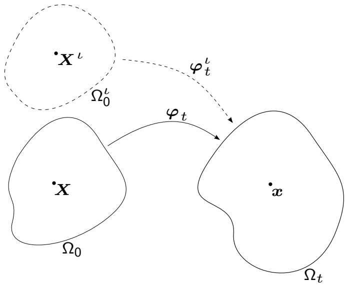


Reference quantities:

ρ_0^{ι} – Species concentration
Π^{ι} – Species production rate
$\boldsymbol{M}^{\iota}$ – Species relative flux
$\boldsymbol{V}^{\iota}$ – Species velocity
$\boldsymbol{g}$ – Body force
$\boldsymbol{q}^{\iota}$ – Interaction force
$\boldsymbol{P}^{\iota}$ – Partial first Piola stress

- Mass balance:
$$\frac{\partial \rho_0^{\iota}}{\partial t} = \Pi^{\iota} - \boldsymbol{\nabla}_X \cdot \boldsymbol{M}^{\iota}$$
- Momentum balance:
$$\rho_0^{\iota} \frac{\partial \boldsymbol{V}^{\iota}}{\partial t} = \rho_0^{\iota} (\boldsymbol{g} + \boldsymbol{q}^{\iota}) + \boldsymbol{\nabla}_X \cdot \boldsymbol{P}^{\iota} - (\boldsymbol{\nabla}_X \boldsymbol{V}^{\iota}) \boldsymbol{M}^{\iota}$$
- Growth-related kinematics:
$$\boldsymbol{F} = \boldsymbol{F}^{\mathrm{e}^{\iota}} \boldsymbol{F}^{\mathrm{g}^{\iota}}; \text{ e.g. } \boldsymbol{F}^{\mathrm{g}^{\iota}} = \left(\frac{\rho^{\iota}}{\rho^{\iota}_{0_{\mathrm{ini}}}} \right)^{\frac{1}{3}} \mathbf{1}$$

Looking at things from an Eulerian perspective



Current quantities:

ρ^ι – Species concentration
π^ι – Species production rate
$\bm{m}^\iota$ – Species total flux
$\bm{v}^\iota$ – Species velocity
$\bm{g}$ – Body force
$\bm{q}^\iota$ – Interaction force
$\bm{\sigma}^\iota$ – Partial Cauchy stress

- The notion of a deformation gradient is unnatural for the fluid
- Mass balance:
  $$\frac{\partial \rho^\iota}{\partial t} = \pi^\iota - \bm{\nabla}_x \cdot \bm{m}^\iota$$
- Momentum balance:
  $$\rho^\iota \frac{\partial \bm{v}^\iota}{\partial t} = \rho^\iota \left(\bm{g}^\iota + \bm{q}^\iota\right) + \bm{\nabla}_x \cdot \bm{\sigma}^\iota - \left(\bm{\nabla}_x \bm{v}^\iota\right) \bm{m}^\iota$$

Toward solving the equations

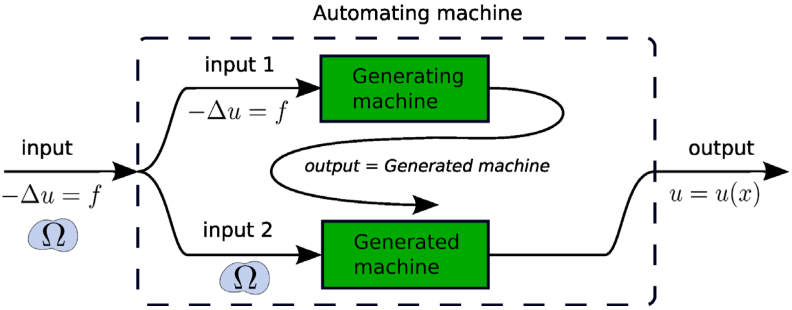
- Turn to the *dissipation inequality* for constitutive relationships to close the system: e.g. Hyperelastic/viscoelastic solids, Newtonian fluids, frictional interaction forces, ...
- Introduce additional constraints like tissue saturation, if needed: $\frac{\left(\rho_0^{\mathrm{s}}/J\right)}{\tilde{\rho}^{\mathrm{s}}} + \frac{\rho^{\mathrm{f}}}{\tilde{\rho}^{\mathrm{f}}} = 1$
- Fix interaction forces or assume microstructural homogenisation to obviate one momentum balance PDE
- An operator-splitting solution scheme (convergence heavily dependent strength of coupling) or fully coupled solution scheme (difficult to implement and extend)

Reintroducing an earlier example

phases, nonlinear, coupled, configurations, BCs, constraints, dynamics

Introducing the FEniCS project

- A collaborative[1] project for the automation of computational mathematical modelling
- Free and open source (`www.fenics.org`)
- Combines generality with efficiency by generating PDE-specific code



[1] Chalmers University of Technology, University of Chicago, Argonne National Laboratory, Toyota Technological Institute, Delft University of Technology, Royal Institute of Technology (KTH), Simula Research Laboratory, Texas Tech, University of Cambridge

A demonstration with Poisson's equation

Strong form:

$$-\nabla^2 u = f$$

Weak form: Find $u \in V$ such that

$$a(v, u) = L(v) \quad \forall v \in \hat{V}$$

where

$$a(v, u) = \int_\Omega \nabla v \cdot \nabla u \, dx$$
$$L(v) = \int_\Omega v f \, dx + \int_{\partial\Omega_N} v g \, ds$$

Working our way up to linear elasticity

Strong form:

$$-\nabla \cdot \sigma(u) = f$$

where

$$\sigma(u) = 2\mu\epsilon(u) + \lambda \mathrm{tr}\, \epsilon(u)\, I$$
$$\epsilon(u) = \frac{1}{2}(\nabla u + (\nabla u)^\top)$$

Weak form: Find $u \in V$ such that

$$a(v, u) = L(v) \quad \forall v \in \hat{V}$$

where

$$a(v, u) = \int_\Omega \nabla v : \sigma(u)\, dx$$
$$L(v) = \int_\Omega v \cdot f\, dx$$

Onto the Navier-Stokes equations for fluid mechanics

Strong form:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\boldsymbol{\nabla} p}{\rho} - \nu \nabla^2 \boldsymbol{u} + (\boldsymbol{\nabla} \boldsymbol{u})\, \boldsymbol{u} = \boldsymbol{f} \,;\; \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

Weak form: Find $(\boldsymbol{u}^{k+1}, p^{k+1}) \in V_u \times V_p$ such that

$$\left(\frac{D\boldsymbol{u}^{k+1}}{\Delta t}, \boldsymbol{v} \right) + \nu (\boldsymbol{\nabla} \boldsymbol{u}^{k+1}, \boldsymbol{\nabla} \boldsymbol{v}) - \left(\frac{p^{\bigstar,k+1}}{\rho}, \nabla \cdot \boldsymbol{v} \right) = (\boldsymbol{g}^{k+1}, \boldsymbol{v}) \quad \forall \boldsymbol{v} \in \hat{V}$$

$$\text{where} \quad \boldsymbol{g}^{k+1} = \boldsymbol{f}^{k+1} - ((\boldsymbol{\nabla} \boldsymbol{u})\, \boldsymbol{u})^{\bigstar,k+1}$$

$$(\nabla \phi, \frac{\nabla \psi^{k+1}}{\rho}) = (\nabla \phi, \frac{D\boldsymbol{u}^{k+1}}{\Delta t}) \quad \forall \phi \in \hat{V}_\phi$$

$$(\frac{p^{k+1}}{\rho}, q) = (\frac{p^{\bigstar,k+1}}{\rho} + \frac{\psi^{k+1}}{\rho} - \nu \nabla \cdot \boldsymbol{u}^{k+1}, q) \quad \forall q \in \hat{V}_p$$

[Guermond and Shen, 2003]

Run into spatial oscillations while solving a BVP

Easily change the scheme to obviate the problem

What is being worked on

- *Automated (symbolic) linearisation of classes of nonlinear forms*
- Improved deforming geometry support
- Improved fluid-structure interaction
- Parallelism for computation on dense meshes describing realistic tissue
- *Adaptive refinement/enrichment toward automation of (goal-oriented) error control*

What else is needed?