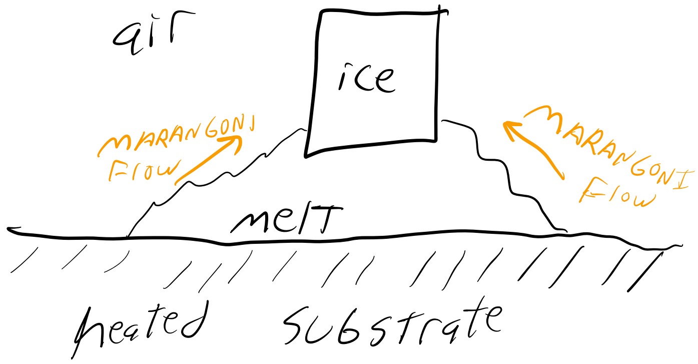
work with: Cody Estebe, Alireza Moradikazerouni, Kourosh Shoele, Mitsuhiro Ohta.

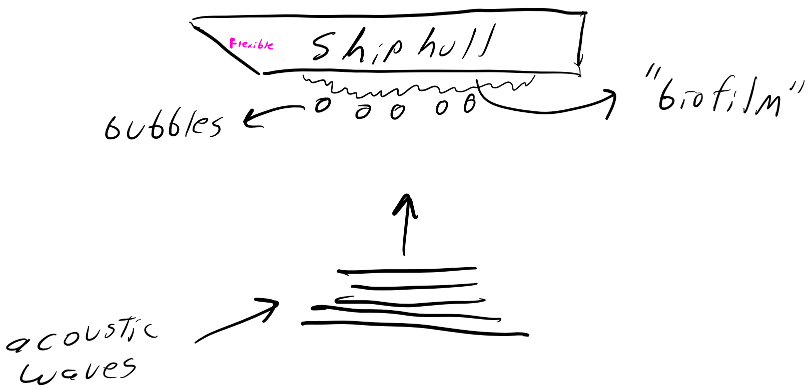
Statement of the problem

1. melting (axisymmetric)

Lappa → rotating flows

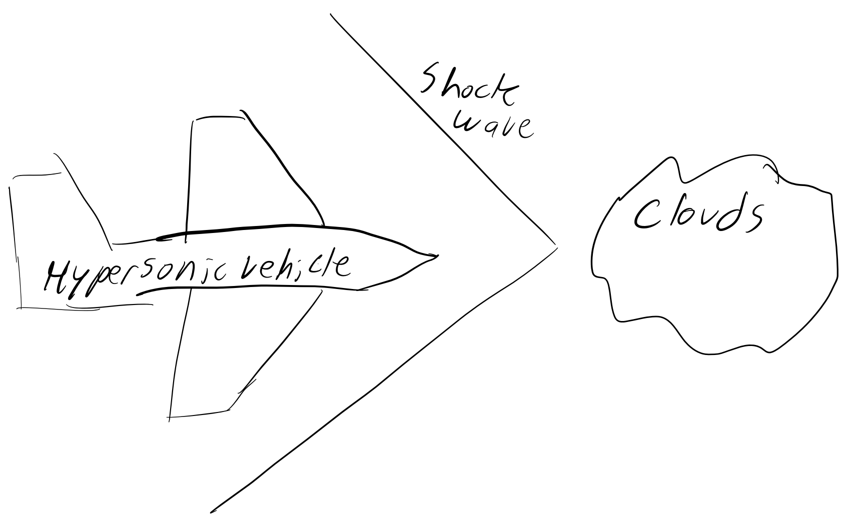


2.

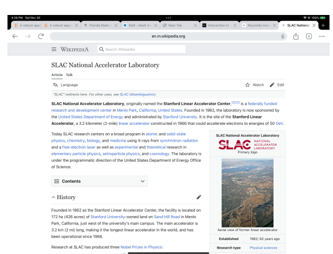


(works for teeth and kidney stones too!)

3.



4. Refrigeration Devices

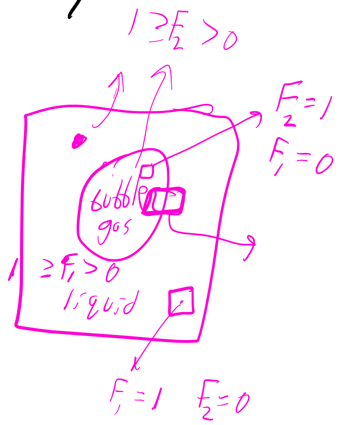


Description of the mathematics

Simplified; no phase change; no dynamic CL model; no Triple point models,

radiation model, electric charge? magnetic field? chemical marangoni effect

$$\begin{pmatrix} F_m \\ \rho_m F_m \\ \rho u \\ \rho_m E_m F_m \end{pmatrix}_t + \vec{\nabla}\cdot \begin{pmatrix} \vec{u} F_m \\ \rho_m F_m \vec{u} \\ \vec{u} \otimes \rho \vec{u} + pI - \tau \\ \left((\rho_m E_m + p)\vec{u} - \vec{u}\cdot\tau - k\nabla T\right) F_m \end{pmatrix} = \begin{pmatrix} F_m \, \vec{\nabla}\cdot\vec{u} \\ 0 \\ \vec{F}_{body} \\ \vec{u}\cdot \vec{F}_{body} F_m \end{pmatrix}$$



$$\tau = \tau_{visc.}(\vec{u}) + \sum_m F_m \tau_m$$

$$\frac{\partial F_m}{\partial t} + \vec{u}\cdot\nabla F_m = 0$$

$$\frac{DF_m}{Dt} = 0$$

← material derivative

$$\tau_{visc.}(\vec{u}) = 2\mu\left(D - \frac{Tr(D)}{Dim}\right)$$

$$D = \frac{\nabla\vec{u} + \nabla\vec{u}^T}{2}$$

$$Dim = 2 \text{ or } 3$$

$$\rho = \sum_m \rho_m F_m$$

$$\mu = \sum_m \mu_m F_m$$

$$\rho_m E_m = \rho_m e_m + \frac{1}{2}\rho_m |\vec{u}|^2$$

$$e_m = c_{v,m} T$$

$$p = p(\rho, e) \quad \text{if compressible}$$

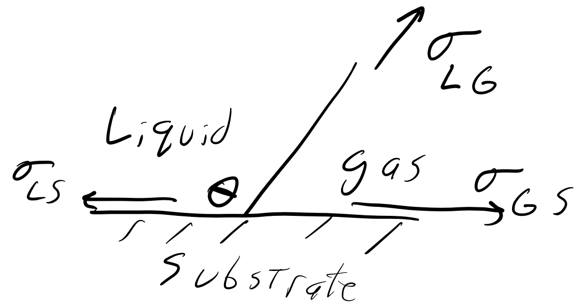
$$\vec{\nabla}\cdot\vec{u} = 0 \quad \text{if incompressible}$$

$$\left[\vec{n}\cdot(pI - \tau)\cdot\vec{n}\right]_{m_1} - \left[\vec{n}\cdot(pI - \tau)\cdot\vec{n}\right]_{m_2} = \sigma_{m_1,m_2} \kappa_{m_1}$$

$$\vec{n}_m = \frac{\vec{\nabla}\phi_m}{|\vec{\nabla}\phi_m|} \qquad \kappa_{m_1} = \vec{\nabla}\cdot\vec{n}_{m_1}$$

$$\left[\vec{n}\cdot\tau\cdot\vec{T}\right]_{m_1} + \left[\vec{n}\cdot\tau\cdot\vec{T}\right]_{m_2} = 0$$

THINC



$$\underbrace{\sigma_{LG}\cos\theta}_{\text{static angle}} + \sigma_{LS} = \sigma_{GS}$$

$\vec{x}(\vec{X}, T)$

Elastic material:

$$\Upsilon_m = G_m B_m$$

$G_m \equiv$ shear modulus

$$B_m = \underset{\sim}{F}_m \underset{\sim}{F}_m^T$$

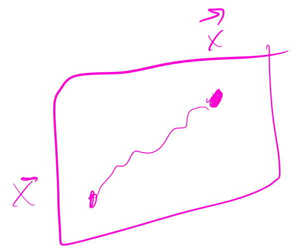
Cauchy Green Strain Tensor

Deformation tensor

$$\underset{\sim}{F}_m = \frac{\partial \vec{x}}{\partial \vec{X}}$$

current position (Eulerian coordinate)

Lagrangian variable



$$\frac{\partial B_m}{\partial t} + \vec{u} \cdot \nabla B_m = \left(\vec{\nabla}\vec{u}\right)^T B_m + B_m\left(\vec{\nabla}\vec{u}\right)$$

$$\frac{\partial B_m}{\partial T} + \nabla \cdot \left(\vec{u} B_m\right) = \left(\nabla \cdot \vec{u}\right) B_m + \left(\vec{\nabla}\vec{u}\right)^T B_m + B_m\left(\vec{\nabla}\vec{u}\right)$$

$$B = \begin{pmatrix} B^{(xx)} & B^{(xy)} & B^{(xz)} \\ B^{(xy)} & B^{(yy)} & B^{(yz)} \\ B^{(xz)} & B^{(yz)} & B^{(zz)} \end{pmatrix}$$

Reynolds transport theorem

In differential calculus, the **Reynolds transport theorem** (also known as the Leibniz–Reynolds transport theorem), or simply the **Reynolds theorem**, named after Osborne Reynolds (1842–1912), is a three-dimensional generalization of the Leibniz integral rule. It is used to recast time derivatives of integrated quantities and is useful in formulating the basic equations of continuum mechanics.

Consider integrating $\mathbf{f} = \mathbf{f}(\mathbf{x},t)$ over the time-dependent region $\Omega(t)$ that has boundary $\partial\Omega(t)$, then taking the derivative with respect to time:

$$\frac{d}{dt}\int_{\Omega(t)} \mathbf{f}\, dV.$$

If we wish to move the derivative into the integral, there are two issues: the time dependence of $\mathbf{f}$, and the introduction of and removal of space from Ω due to its dynamic boundary. Reynolds transport theorem provides the necessary framework.

Contents

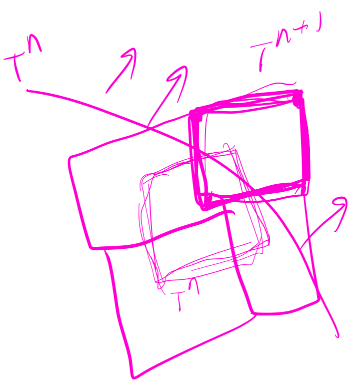
General form

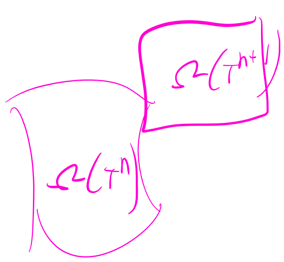
Reynolds transport theorem can be expressed as follows:[1][2][3]

$$\frac{d}{dt}\int_{\Omega(t)} \mathbf{f}\, dV = \int_{\Omega(t)} \frac{\partial \mathbf{f}}{\partial t}\, dV + \int_{\partial\Omega(t)} (\mathbf{v}_b \cdot \mathbf{n})\, \mathbf{f}\, dA$$

in which $\mathbf{n}(\mathbf{x},t)$ is the outward-pointing unit normal vector, $\mathbf{x}$ is a point in the region and is the variable of integration, dV and dA are volume and surface elements at $\mathbf{x}$, and $\mathbf{v}_b(\mathbf{x},t)$ is the velocity of the area element (*not* the flow velocity). The function $\mathbf{f}$ may be tensor-, vector- or scalar-valued.[4] Note that the integral on the left hand side is a function solely of time, and so the total derivative has been used.

Form for a material element



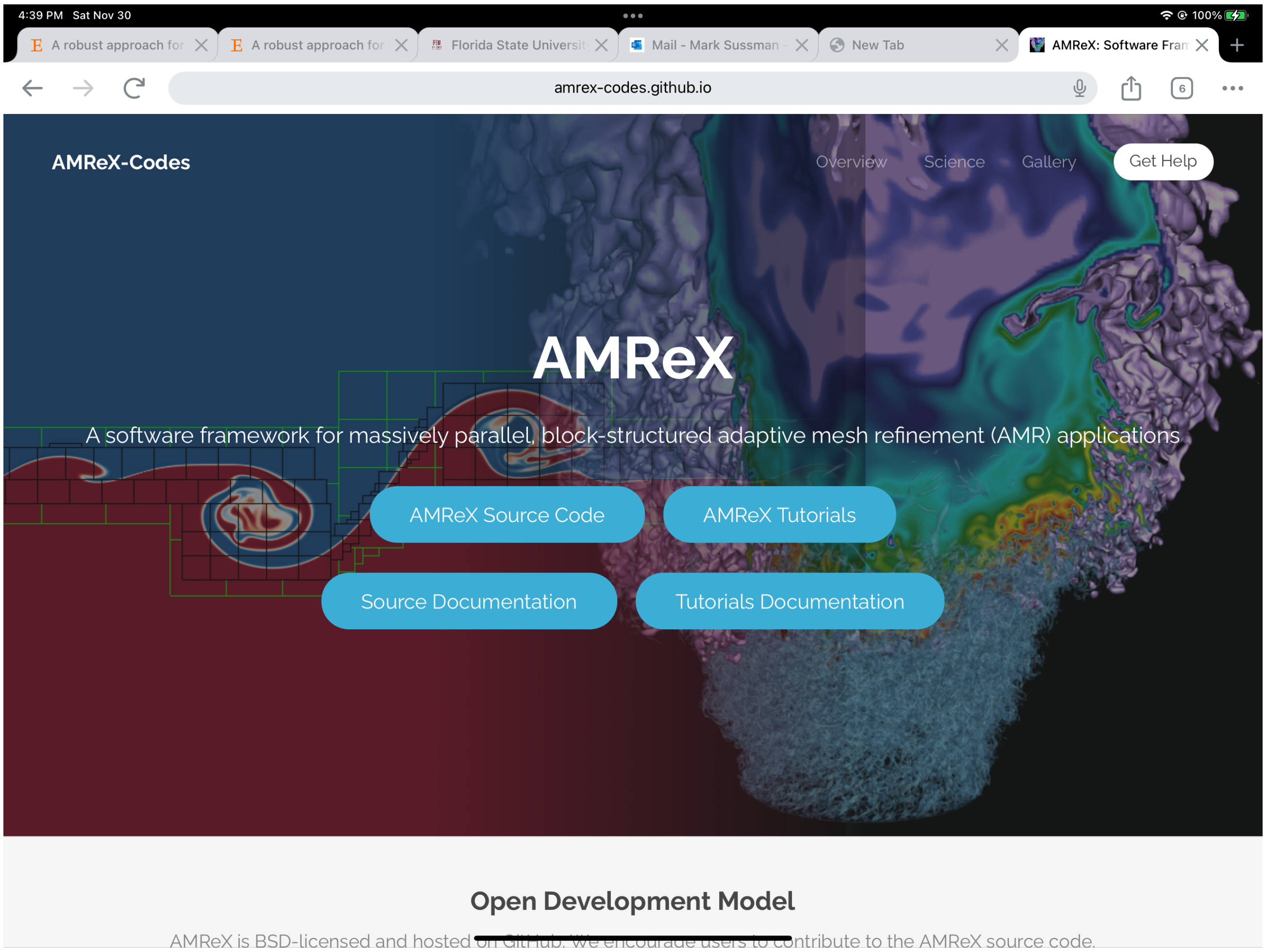


cell integrated
Semi-Lagrangian
method

Mikhail Shashkov

LANL

Algorithm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A robust approach for
A robust approach for
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Journal of Computational Physics 230 (2011) 596–627

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

ELSEVIER

A full Eulerian finite difference approach for solving fluid–structure coupling problems

we do finite volume

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ARTICLE INFO

Article history:
Received 26 February 2010
Received in revised form 30 August 2010
Accepted 15 September 2010
Available online 15 October 2010

Keywords:
Fluid–structure interaction
Finite difference method

ABSTRACT

A new simulation method for solving fluid–structure coupling problems has been developed. All the basic equations are numerically solved on a fixed Cartesian grid using a finite difference scheme. A volume-of-fluid formulation [Hirt, Nichols, J. Comput. Phys. 39 (1981) 201], which has been widely used for multiphase flow simulations, is applied to describing the multi-component geometry. The temporal change in the solid deformation is described in the Eulerian frame by updating a left Cauchy-Green deformation tensor, which is used to express constitutive equations for nonlinear Mooney–Rivlin materials. In this paper, various verifications and validations of the present full Eulerian method, which solves the fluid

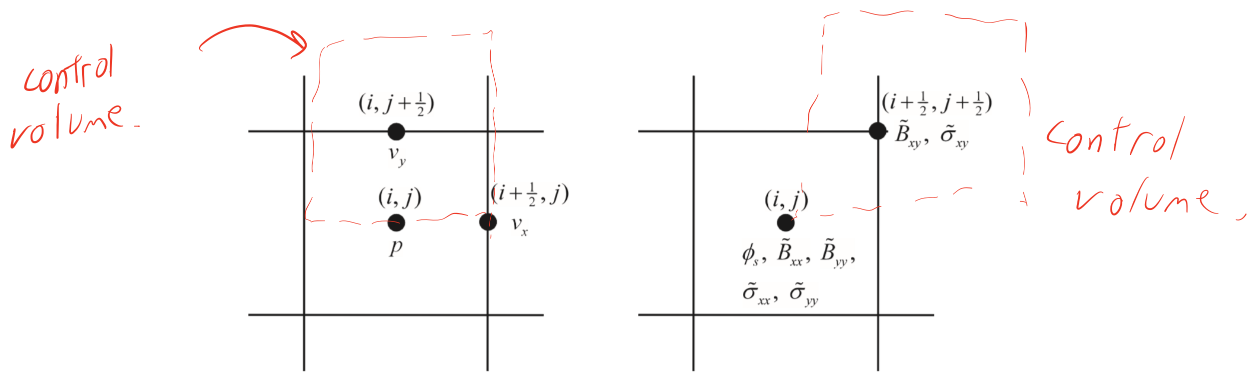
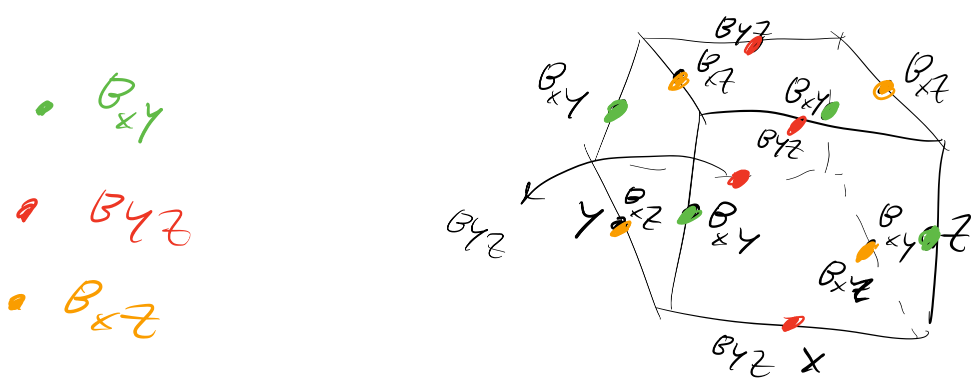


Fig. 4. Schematic figure of computational grid with the mesh size of $\Delta_x \times \Delta_y$, here $\Delta_x = \Delta_y$. (a) Left panel: Definition points of the velocity components v_x, v_y, and the pressure p. (b) Right panel: Definition points of the solid volume fraction ϕ_s, the stress components $\tilde{\sigma}_{xx}, \tilde{\sigma}_{yy}, \tilde{\sigma}_{xy}$, and the modified left Cauchy-Green deformation components $\tilde{B}_{xx}, \tilde{B}_{yy}, \tilde{B}_{xy}$.



Received: 28 December 2019 | Revised: 29 February 2020 | Accepted: 21 March 2020
DOI: 10.1002/fld.4836

RESEARCH ARTICLE

WILEY

Interaction of a deformable solid with two-phase flows: An Eulerian-based numerical model for fluid-structure interaction using the level contour reconstruction method

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Funding information
GENCI(Grand Equipement National de Calcul Intensif), Grant/Award Number: Grant 2019 A0062B06721; National Research Foundation, Grant/Award Number: 2020R1A2C1003822; Centre National de la Recherche Scientifique

Summary
We describe the formulation of a method for fluid-structure interaction involving the coupling of moving and/or flexible solid structures with multiphase flows in the framework of the Level Contour Reconstruction Method. We present an Eulerian-based numerical procedure for tracking the motion and interaction of a liquid-gas interface with a fluid-solid interface in the Lagrangian frame together with the evaluation of the fluid transport equations coupled to those for the solid transport, namely the left Cauchy-Green strain tensor field, in the Eulerian frame. To prevent excessive dissipation due to the convective nature of the solid transport equation, a simple incompressibility constraint for the strain field is enforced. A single grid structure is used for both the fluid and solid phases which allows for a simple and natural coupling of the fluid and solid dynamics. Several benchmark tests are performed to show the accuracy of the numerical method and which demonstrate accurate results compared to several of those in the existing literature. In particular we show that surface tension effects including contact line dynamics on the deforming solid phase can be properly simulated. The three-phase interaction of a droplet impacting on a flexible cantilever is investigated in detail. The simulations follow the detailed motion of the droplet impact (and subsequent deformation, breakup, and fall trajectory) along with the motion of the deformable solid cantilever due to its own weight as well as due to the force of the droplet impact.

KEYWORDS
Eulerian-based formulation, fluid-structure interaction, front-tracking method, multiphase flow, numerical simulation, solid stress

For simplicity and without loss of generality we focus on the 2D formulation so that we can write the deformation tensor, **F**, as

$$F = \begin{pmatrix} \frac{\partial x}{\partial X} & \frac{\partial x}{\partial Y} \\ \frac{\partial y}{\partial X} & \frac{\partial y}{\partial Y} \end{pmatrix}, \tag{6}$$

where (x,y) is the current and (X,Y) is the reference or original location of the material. The 3D formulation is straightforward and key elements are provided in the appendix. Most FEMs evaluate the deformation tensor field, **F**, directly by tracking Lagrangian element motion.

In this study, we evaluate the left Cauchy-Green strain tensor field directly without computing the deformation tensor field, **B**, using the transport equation provided by Sugiyama et al.[17] First, we define a modified left Cauchy-Green strain tensor, **C**, instead of **B** in the same way as Sugiyama et al[17] for numerical stability as:

$$\mathbf{C} = {H_s}^{0.5}\mathbf{B}. \tag{7}$$

The transport equation for the modified left Cauchy-Green strain tensor is time advanced according to:

$$\frac{\partial \mathbf{C}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{C} = \nabla \mathbf{u}^T \cdot \mathbf{C} + \mathbf{C} \cdot \nabla \mathbf{u}. \tag{8}$$

In this way, the stress field is confined to the solid region and provides a smoother transition from solid to fluid in order to prevent sudden changes in the stress evolution. Using Equations (4) and (7), Equation (3) is now:

$$\widetilde{\boldsymbol{\sigma}} = [\mu_f + (\mu_s - \mu_f)H_s](\nabla \mathbf{u} + \nabla \mathbf{u}^T) + H_s \widetilde{\boldsymbol{\sigma}}_{sh} = \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T) + G{H_s}^{0.5}\mathbf{C}. \tag{9}$$

The material property fields can be described using two Heaviside functions as follows:

$$\begin{aligned} b &= (1 - H_s)b_f + H_s b_s \\ b_f &= (1 - H_f)b_l + H_f b_g, \end{aligned} \tag{10}$$

where, b represents density or viscosity fields with the subscripts s, f, l, g standing for solid, fluid, liquid or gas, respectively. The two Heaviside functions, H_s and H_f, can be computed from the two distance functions distinguishing the fluid-solid (ϕ_s) or the liquid-gas (ϕ_f) respectively.

$$\begin{cases} H_s(\phi_s) = 1, & \phi_s \geq 0 \\ H_s(\phi_s) = 0, & \phi_s < 0 \end{cases} \quad \begin{cases} H_f(\phi_f) = 1, & \phi_f \geq 0 \\ H_f(\phi_f) = 0, & \phi_f < 0 \end{cases}. \tag{11}$$

2.3 | Solution procedure

The detailed method for solving the Navier-Stokes equations for the fluid can be found in References 24-28. Here we briefly describe the basic procedure for the fluid and then focus on the solution for solid deformation. We solve the fluid flow and solid motion separately. For the fluid, the standard incompressible Navier-Stokes equations are:

(12)

we try something else,
also we preserve volume exactly,
any # of elastic materials,
solvability condition automatic on AMR grid,
scalable algorithm,

monolithic approach ?

$$\frac{\vec{\xi}^{n+1}-\vec{\xi}^{n}}{\Delta T}=\vec{F}(\vec{\xi}^{n+1},T^{n+1})$$

$$\frac{\begin{pmatrix} F_m \\ \rho_m F_m \\ \rho u \\ \rho_m E_m F_m \end{pmatrix}^{n+1}-\begin{pmatrix} F_m \\ \rho_m F_m \\ \rho u \\ \rho_m E_m F_m \end{pmatrix}^{n}}{\Delta T} \leftarrow \begin{pmatrix} F_m \\ \rho_m F_m \\ \rho u \\ \rho_m E_m F_m \end{pmatrix}_T + \vec{\nabla}\cdot\begin{pmatrix} \vec{u}F_m \\ \rho_m F_m \vec{u} \\ \vec{u}\otimes\rho\vec{u}+pI-\tau \\ (\rho_m E_m + p)\vec{u}-\vec{u}\cdot\tau - k\nabla T) F_m \end{pmatrix}^{n+1} = \begin{pmatrix} F_m\ \vec{\nabla}\cdot\vec{u} \\ 0 \\ \vec{F}_{body} \\ \vec{u}\cdot\vec{F}_{body} F_m \end{pmatrix}^{n+1}$$

pros: unconditionally stable

cons: not robust; nonlinear problem
existance & uniqueness?
sensitivity to initial guess?

$$\tau^{n+1}=\left(\tau_{visc.}(\vec{u})+\sum_m F_m \tau_m\right)^{n+1}$$

$$\left(\tau_{visc.}(\vec{u})\right)^{n+1}=\left(2\mu\left(D-\frac{Tr(D)}{Dim}\right)\right)$$

$$D^{n+1}=\left(\frac{\nabla\vec{u}+\nabla\vec{u}^T}{2}\right)^{n+1}$$

$$Dim = 2 \text{ or } 3$$

$$(\rho)^{n+1}=\left(\sum_m \rho_m F_m\right)^{n+1}$$

$$\mu^{n+1}=\left(\sum_m \mu_m F_m\right)^{n+1}$$

$$(\rho_m E_m)^{n+1}=\left(\rho_m e_m+\frac{1}{2}\rho_m|\vec{u}|^2\right)^{n+1}$$

$$(e_m)^{n+1}=(c_{v,m}T)^{n+1}$$

$$p^{n+1}=p(\rho^{n+1},e^{n+1}) \quad \text{if compressible}$$

$$\vec{\nabla}\cdot\vec{u}^{n+1}=0 \quad \text{if incompressible}$$

$$\left[\vec{n}\cdot(pI-\tau)\cdot\vec{n}\right]_{m_1}^{n+1}-\left[\vec{n}\cdot(pI-\tau)\cdot\vec{n}\right]_{m_2}^{n+1}=\left(\sigma_{m_1m_2}K_{m_1}\right)^{n+1}$$

$$\frac{B_m^{n+1}-B_m^{n}}{\Delta T}$$

$$(\vec{n}_m)^{n+1}=\left(\frac{\vec{\nabla}\phi_m}{|\vec{\nabla}\phi_m|}\right)^{n+1} \qquad K_{m_1}^{n+1}=(\vec{\nabla}\cdot\vec{n}_m)^{n+1}$$

$$\left[\vec{n}\cdot\tau\cdot\vec{T}\right]_{m_1}^{n+1}+\left[\vec{n}\cdot\tau\cdot\vec{T}\right]_{m_2}^{n+1}=0$$

$$\frac{\partial B_m}{\partial T}+\left(\nabla\cdot(\vec{u}B_m)\right)^{n+1}=\left((\nabla\cdot\vec{u})B_m\right)^{n+1}+\left((\vec{\nabla}\vec{u})^T B_m\right)^{n+1}+\left(B_m(\vec{\nabla}\vec{u})\right)^{n+1}$$

Explicit Approach?

$$\frac{\vec{\zeta}^{\,n+1} - \vec{\zeta}^{\,n}}{\Delta T} = \vec{F}(\vec{\zeta}^{\,n}, T^n)$$

pros:
very robust

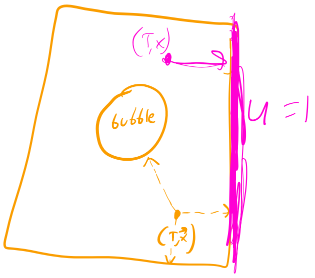
cons: volume not preserved

topic for another day.
Level set method?
VOF?
MOF?
phase field method?
SPH?

material boundaries diffuse over Time.

Physically informed Neural Networks

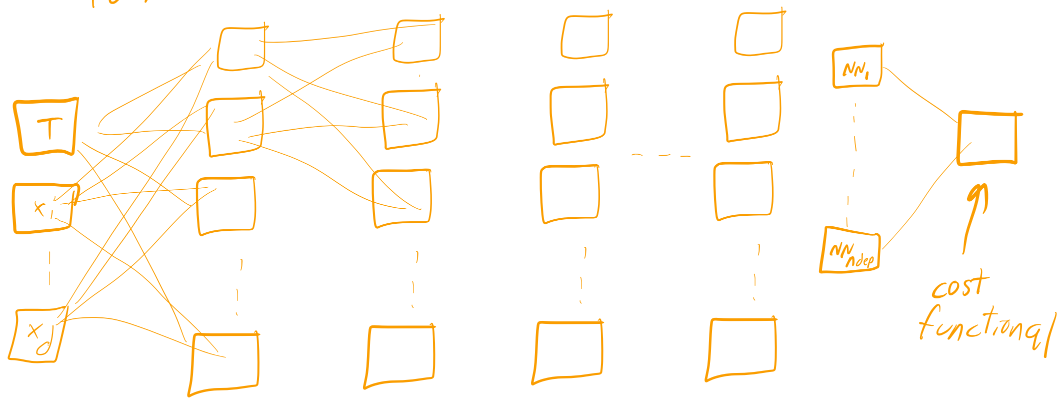
PINN approach



$$\vec{m}_j\left(\vec{u}(t,\vec{x})\right) = \vec{F}_j(t,\vec{x})$$

functional

$j = 0,1,2,3,\dots,N_{functionals}$



$$C\left(NN(T,\vec{x},\vec{\theta}),\vec{\theta}\right) = \sum_j w_j \left\| \vec{m}_j\left(NN(T,\vec{x},\vec{\theta})\right) - \vec{F}_j(t,\vec{x}) \right\|^2$$

$$+\, w_\theta \|\theta\|^2$$

regularization (can iterate on the I.C. using this term)

Some possible functionals (m_j):

(i) vorticity-velocity formulation

(ii) integral formulation vs. pointwise

(iii) Reynolds' transport Theorem:

Reynolds transport theorem can be expressed as follows:[1][2][3]

$$\frac{d}{dt}\int_{\Omega(t)} \mathbf{f}\,dV = \int_{\Omega(t)} \frac{\partial \mathbf{f}}{\partial t}\,dV + \int_{\partial\Omega(t)} (\mathbf{v}_b\cdot\mathbf{n})\,\mathbf{f}\,dA$$

(IV) enforce conservation laws.

(V) preservation of enstrophy

note:

→ AMR is Trivial with PINN

→ results from the past can be used as I.C. in the future. Also used for improving the cost function (enhanced regularization)

Divide and Conquer

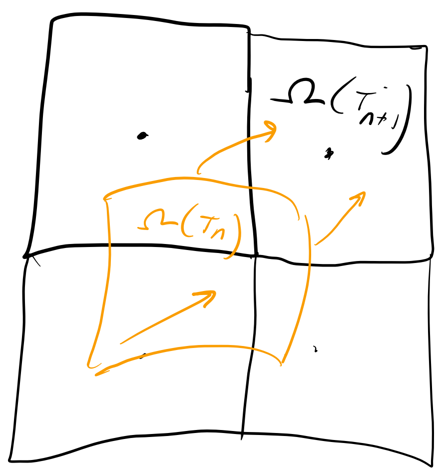
(A) CISL ADVECTION

Reynolds transport theorem can be expressed as follows:[1][2][3]

$$\frac{d}{dt}\int_{\Omega(t)} \mathbf{f}\,dV = \int_{\Omega(t)} \frac{\partial \mathbf{f}}{\partial t}\,dV + \int_{\partial\Omega(t)} (\mathbf{v}_b \cdot \mathbf{n})\,\mathbf{f}\,dA$$

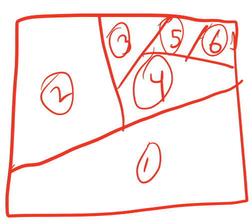
$$\begin{pmatrix} F_m \\ \rho_m F_m \\ \rho u \\ \rho_m E_m F_m \end{pmatrix}_t + \vec{\nabla}\cdot\begin{pmatrix} \vec{u} F_m \\ \rho_m F_m \vec{u} \\ \vec{u}\otimes\rho\vec{u} \\ (\rho_m E_m)\vec{u} F_m \end{pmatrix} = 0$$

$$\frac{\partial B_m}{\partial T} + \nabla\cdot(\vec{u} B_m) = 0$$



nested dissection,

e.g. 6 materials



(B) expansion terms & others,

$$(F_m)_T = F_m (\nabla \cdot \vec{u})^n$$

explicit

$$\frac{\partial B_m}{\partial T} = (\nabla \cdot \vec{u}) B_m + (\nabla u)^T B_m + B_m (\nabla u)$$

(C)

For J = 1 -- $N_{material}$
 save current state
endfor

For j = 1, -- , $N_{elastic}$ + 1

restore non-elastic state(s)

for i = J, - - , $N_{elastic}$
 restore m_i state
endfor

for i = 1, --, J
 fix m_i state
endfor

for i = 1 -- J
 extrapolate B_{m_i}, $\vec{u}_{m_i}$, ρ_{m_i}, μ_{m_i} into the
 non-elastic regions; band size = 2Δx
endfor

viscosity: $(\rho\vec{u})_T - \nabla \cdot \tau_{visc} = 0$ implicit (non-fixed regions)

for i = J, --, $N_{elastic}$
 $(\rho\vec{u})_T - \nabla \cdot (F_{m_i} \tau_{m_i}) = 0$ explicit
end

if J ≤ $N_{elastic}$
 $(\rho\vec{u})_T + \nabla \cdot (pI) = 0$ "projection"
else
 $(\rho\vec{u})_T + \nabla \cdot (pI) = -\sigma k \nabla H$
endif

non-fixed regions

endfor

remove null space

$$\begin{cases} \nabla \cdot \dfrac{\nabla p}{\rho} = F \\ \nabla p \cdot n = 0 \quad \vec{x} \in \partial\Omega \end{cases}$$

Neumann

$(\rho u)_t + \nabla \cdot (pI) = 0$

$$A^T = A$$

$$\begin{pmatrix} A & v \\ v^T & 0 \end{pmatrix} x^* = \begin{pmatrix} \vec{b} \\ 0 \end{pmatrix}$$

Suppose $x^* = \begin{pmatrix} \vec{v} \\ \alpha \end{pmatrix}$

$$\Rightarrow A^* x^* = \begin{pmatrix} \alpha \vec{v} \\ v^T v \end{pmatrix} \neq \vec{0}$$

$Aw \cdot v = w \cdot A^T v$
$= 0$

pick $\vec{w}$ $\ni$ $\vec{w} \cdot \vec{v} = \vec{0}$

only when
$\vec{w} = \vec{0}$
$\alpha = 0$

or $x^* = \begin{pmatrix} \vec{w} \\ \alpha \end{pmatrix} \Rightarrow A x^* = \begin{pmatrix} A\vec{w} + \alpha \vec{v} \\ v^T \vec{w} \end{pmatrix} = \vec{0}$

$= 0$

results

https://www.math.fsu.edu/~sussman/PLICmelt1.mp4

https://www.math.fsu.edu/~sussman/PARTICLEmelt1.mp4

https://www.math.fsu.edu/~sussman/REFCENmelt1.mp4

https://www.math.fsu.edu/~sussman/PLICmelt2.mp4

https://www.math.fsu.edu/~sussman/PLICbiofilm.mp4

https://www.math.fsu.edu/~sussman/PLICbiofilm100.mp4

conclusions

1. contrary to what one might think, one can (conditionally) stably discretize elastic material force explicitly in time and tie it together with other interacting materials.

2. we are still in the verification, and validation phase.

3. simulations take a long time, but we argue that it is currently the "Least worst" solution to the given problem.

4. The PINN approach is promising considering that it has taken ~20 years of development time with the present approach. You will have to consult my past students & postdocs to see what their feelings on the matter are.