Discretization Techniques for Surface Tension Forces in Fully Conservative Two-Phase Flow Finite Volume Methods

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Outline

- Basic Concepts (Waidmann)

- Conservative Continuous Surface Stress Approach (Waidmann)

- Conservative Well-Balanced Sharp Interface Approach (Gerber)

- Summary (Gerber)
Basic Concepts

- fully conservative Finite Volume DNS
  - solving space-time integral conservation laws
  - conservative discretization

- Cartesian grid (*) (2d & 3d)

- sharp interface (*) [*]

- projection type predictor-corrector method

- C++ implementation built on SAMRAI (AMR, parallel), LLNL

(*) ⇒ cut grid cells at the sharp interface

[*] ⇒ jumps (ρ, p, μ, D ...) at the sharp interfaces
Basic Concepts

governing equations, leading order system\textsuperscript{[1]}, zero Mach number limit

\begin{align*}
\text{mass} : & \quad \frac{d}{dt} \int_{\Omega} \rho \, dV = - \int_{\partial \Omega} \left( \rho \theta \boldsymbol{u} \cdot \boldsymbol{n} \right) \left( \frac{1}{\theta} \right) \, dS \\
\text{spec} : & \quad \frac{d}{dt} \int_{\Omega} \rho Y_s \, dV = - \int_{\partial \Omega} \left( \rho \theta \boldsymbol{u} \cdot \boldsymbol{n} \right) \left( \frac{Y_s}{\theta} \right) \, dS - \int_{\partial \Omega} \mathbf{j}_s \cdot \boldsymbol{n} \, dS + \int_{\Omega} \hat{\rho}_s \, dV \\
\text{mom} : & \quad \frac{d}{dt} \int_{\Omega} \rho \boldsymbol{u} \, dV = - \int_{\partial \Omega} \left( \rho \theta \boldsymbol{u} \cdot \boldsymbol{n} \right) \left( \frac{\boldsymbol{u}}{\theta} \right) \, dS + \int_{\partial \Omega} \mathbf{T} \cdot \mathbf{n} \, dS + \int_{\Omega} \rho \mathbf{g} \, dV - \int_{\partial \Omega} \rho^{(2)} \boldsymbol{n} \, dS + \int_{\partial \Omega \cap \Gamma(t)} \sigma \boldsymbol{t} \, d\Gamma \\
\text{en} : & \quad 0 = - \int_{\partial \Omega} \left( \rho \theta \alpha \cdot \boldsymbol{n} \right) \, dS + \int_{\partial \Omega \cap \Gamma(t)} \rho \theta D \, dV \\
\text{with} & \quad \int_{\Omega} \rho \theta D \, dV = - \frac{d \rho^{(0)}}{dt} \int_{\Omega} \frac{\theta}{c^2} \, dV + \int_{\Omega} \left( \frac{\theta}{c^2} \Xi \left[ \nabla \cdot \mathbf{q} + \sum_s \mathbf{j}_s \cdot \nabla h_s + \sum_s \Delta h_s \hat{\rho}_s \right] \right) \, dV \\
\text{vof} : & \quad \frac{d}{dt} \int_{\Omega} \rho \theta \alpha \, dV = - \int_{\partial \Omega} \left( \rho \theta \alpha \cdot \boldsymbol{n} \right) \alpha \, dS \\
\text{ls} : & \quad \frac{d}{dt} \mathbf{G} = - \mathbf{u} \cdot \nabla \mathbf{G} \quad \text{[2]} \\
\text{surf} : & \quad \frac{d}{dt} \int_{\Omega \cap \Gamma(t)} \chi \, dS = - \int_{\partial \Omega \cap \Gamma(t)} \chi \cdot \mathbf{n} \, d\Gamma + \int_{\Omega \cap \Gamma(t)} D_{\Gamma(t)} \nabla \mathbf{r}_\Gamma \cdot \chi \, d\Gamma + \int_{\Omega \cap \Gamma(t)} \mathbf{j}_\Gamma \cdot \mathbf{n}_{\Gamma(t)} \, dS
\end{align*}

\textsuperscript{[2]} Waidmann et. al.; Proceedings in Mathematics & Statistics 77 (2014)
Continuous Surface Stress Approach

space-time integral momentum equation at zero velocity and gravity

\[
\rho \mathbf{u}^{n+1} - \rho \mathbf{u}^n = - \int_{t^n}^{t^{n+1}} \int_{\partial \Omega} \rho^{(2)} \mathbf{n} \, dS \, dt + \int_{t^n}^{t^{n+1}} \int_{\partial \Omega \cap \Gamma} \mathbf{t} \, d/ \, dt
\]

\[
\int_{\partial \Omega \cap \Gamma} \sigma \mathbf{t} \, d/ = \int_{\partial \Omega \cap \Gamma} \mathbf{T}^\sigma \cdot \mathbf{t} \, d/ = \int_{\Omega \cap \Gamma} \nabla \cdot \mathbf{T}^\sigma \, dS = \int_{\Omega} \nabla \cdot (\mathbf{T}^\sigma \delta_G) \, dV = \int_{\partial \Omega} \mathbf{T}^\sigma \delta_G(\mathbf{x}, t) \cdot \mathbf{n} \, dA
\]

\[
\mathbf{T}^\sigma := \sigma (\mathbf{I} \mathbf{d} \mathbf{d} - \mathbf{n}_G \otimes \mathbf{n}_G)
\]

Continuous Surface Stress Approach

space-time integral momentum equation at zero velocity and gravity
Continuous Surface Stress Approach

Continuous Surface Stress \[2\] [3] [4] [5]

\[
\rho \bar{u}^{n+1} = \rho \bar{u}^n - \int_{t^n}^{t^{n+1}} \int_{\partial \Omega} p^{(2)} \tilde{n} \, dA \, dt + \int_{t^n}^{t^{n+1}} \int_{\Omega} \tilde{f}_\sigma \, dV \, dt
\]

\[
\rho \bar{u}^{n+1} = \rho \bar{u}^n - \int_{t^n}^{t^{n+1}} \int_{\partial \Omega} \left( p^{(2)} \mathbf{I} - T^\sigma_\Gamma \delta(d_\Gamma(\tilde{x}, t)) \right) \cdot \tilde{n} \, dA \, dt
\]

\( T^\sigma_\Gamma := \sigma (\mathbf{I} \mathbf{d} - \tilde{n}_\Gamma \circ \tilde{n}_\Gamma) \)

Advantages:

- pressure and surface stress tensor treated as a single unit \([9]\)
- no explicit curvature evaluation (no discrete second derivatives)
- fully conservative momentum equation \(\rightarrow\) fluxes
- arbitrary locally varying surface tension coefficient \(\sigma\)

\[9\] Francois et al., A balanced-force algorithm ... , JCP 213, 2006
Continuous Surface Stress Approach

Discretization

\[
\int_{t^n}^{t^{n+1}} \int_{\partial\Omega} \mathbf{T}_f^\sigma \delta_d \cdot \vec{n} \, dA \, dt = \int_{t^n}^{t^{n+1}} \int_{\partial\Omega} \vec{f}_A \, \delta_d \, dA \, dt \approx \int_{t^n}^{t^{n+1}} \int_{\partial\Omega} \vec{f}_A \frac{\nabla \sigma}{|\nabla \sigma|} \delta^{[1]}_{\epsilon|\nabla \sigma|} (G) \, dA \, dt
\]

(2)

force on control volume boundary:

\[
\vec{f}_A := \mathbf{T}_f^\sigma \cdot \vec{n} = \sigma (\mathbf{I} - \vec{\eta} \circ \vec{\eta}) \cdot \vec{n} = \sigma (\vec{n} - \vec{\eta} \cdot (\vec{\eta} \cdot \vec{n})) = \sigma \left( \vec{n} - \frac{\nabla G}{|\nabla G|} \left( \frac{\nabla G}{|\nabla G|} \cdot \vec{n} \right) \right)
\]

(3)

Approximation of Dirac distribution for non-distance functions \( G \):

\[
\delta_d = \delta (\vec{x} - \vec{x}_f) = \delta^{[1]} (d) \approx \delta^{[1]} \left( \frac{G}{|\nabla G|} \right) \approx \delta^{[1]}_{\epsilon} \left( \frac{G}{|\nabla G|} \right)
\]

(4)

\[
\delta^{[1]}_{\epsilon} \left( \frac{G}{|\nabla G|} \right) := \frac{1}{\epsilon} \psi_{\epsilon} \left( \frac{G}{|\nabla G|} \right) = \frac{|\nabla G|}{\epsilon |\nabla G|} \psi_{\epsilon|\nabla G|} (G) = |\nabla G| \delta^{[1]}_{\epsilon|\nabla G|} (G)
\]

(5)

1D linear hat function:

\[
\psi_{\epsilon} (\xi) := \begin{cases} 
1 - \frac{1}{\epsilon} \frac{|\xi|}{\epsilon} & |\xi| \leq \epsilon \\
0 & |\xi| > \epsilon
\end{cases}
\]

(6)
Continuous Surface Stress Approach

space-time integral momentum equation at zero velocity and gravity
Continuous Surface Stress Approach
Discretization, 2D

\[
\int_{t^n}^{t^{n+1}} \int_{\partial \Omega} \mathbf{T}^g_\Gamma \delta \mathbf{n} \, dA \, dt = \int_{t^n}^{t^{n+1}} \int_{\partial \Omega} \tilde{t}_A \left| \nabla G \right| \delta^{[1]}_{\epsilon \left| \nabla G \right|} (G) \, dA \, dt \\
= \int_{t^n}^{t^{n+1}} \int_{\partial \Omega} \tilde{t}_A \left| \nabla G \right| \frac{1}{\epsilon \left| \nabla G \right|} \left( 1 - \frac{\text{sgn}(G) \ G}{\epsilon \left| \nabla G \right|} \right) \, dA \, dt \\
= \int_{t^n}^{t^{n+1}} \int_{\partial \Omega} \tilde{E}_A \left( 1 - \text{sgn}(G) \ (G \ E_\epsilon) \right) \, dA \, dt \\
:= \tilde{F}_{F,E} \\
:= \tilde{G}_{G,E}
\]

\[
2D \sum_{\tau} \sum_{s=0}^{S_\tau} \int_{\eta_{\tau,s}(t)}^{n_{\tau}} \int_{\eta_{\tau,s}(t)}^{u_{\tau,s}(t)} \left( \sum_{i=0}^{1} \sum_{j=0}^{1} \tilde{k}_{ij}^{(F)} t^i y^j \right) \left( \sum_{i=0}^{1} \sum_{j=0}^{1} \tilde{g}_{ij}^{(\tau,s)} t^i y^j \right) \, dy \, dt \qquad (7)
\]
Continuous Surface Stress Approach
Discretization, 2D

\[
\int_{t^n}^{t^{n+1}} \int_{\partial \Omega} \mathbf{T}^{\sigma} \delta_d \cdot \vec{n} \, dA \, dt = \sum_{\tau} \sum_{s=0}^{S_{\tau}} \int_{t^{\tau}_s}^{t^{\tau}_{s+1}} \int_{I_{\tau,s}(t)} \left( \sum_{i=0}^{2} \sum_{j=0}^{2} \tilde{q}_{ij} \left( \tilde{k}_{ij}^{(\vec{F})}, \tilde{s}_{ij}^{(\tau,s)} \right) \right) t^i y^j \, dy \, dt
\]

\[
= \sum_{\tau} \left( n_{\tau} - o_{\tau} \right) \frac{1}{2} \sum_{s=0}^{S_{\tau}} \sum_{i=0}^{2} \sum_{j=0}^{2-i} \tilde{w}_{ij}^{(\tau,s)} n_{\tau}^i o_{\tau}^j
\]  

(8)

\[
\tilde{w}_{ij}^{(\tau,s)} := \frac{1}{\tilde{\psi}(i+j)} \sum_{a=0}^{2} \tilde{q}^{(\tau,s)}_{(i+j)a} \tilde{w}^{(\tau,s)}_{ij}
\]

\[
\tilde{w}_{ija}^{(\tau,s)} := \frac{1}{\tilde{\zeta}(i+j)a} \sum_{b=0}^{a+1} \tilde{\varphi}(a+1-b) \tilde{\varphi} bj \mathcal{U}_{ab}
\]

\[
\mathcal{U}_{ab} := (u(n)^{a+1-b} u(o)^b - l(n)^{a+1-b} l(o)^b)
\]

\[
\tilde{q}^{(\tau,s)}_{(a+c)(b+d)} := \frac{1}{4} \left[ \left( \begin{array}{c} 2 \\ a+c \end{array} \right) \left( \begin{array}{c} 2 \\ b+d \end{array} \right) \left( \tilde{s}_{ab}^{(\tau,s)} \tilde{k}_{cd}^{(\vec{F})} + \tilde{s}_{ad}^{(\tau,s)} \tilde{k}_{cb}^{(\vec{F})} + \tilde{s}_{bd}^{(\tau,s)} \tilde{k}_{ca}^{(\vec{F})} + \tilde{s}_{cd}^{(\tau,s)} \tilde{k}_{ba}^{(\vec{F})} \right) \right]
\]
Continuous Surface Stress Approach  
Discretization, 2D

\[ \tilde{\psi}_m := \binom{2 + m}{m} \quad \tilde{\varphi}_{mn} := \binom{m + n}{n} \quad \tilde{\zeta}_{mn} := \binom{2 + m + n}{n} \]
Continuous Surface Stress Approach
First Results, 2D

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Continuous Surface Stress Approach
First Results, 2D
Continuous Surface Stress Approach
First Results, 2D

\[
[p] = \sigma \kappa = \sigma \frac{1}{R}
\]

\[
R := \frac{3}{2}, \quad \sigma(\tilde{x}, t) = \sigma_0 = 1 \quad \rightarrow \quad [p] = \frac{2}{3}
\]
Continuous Surface Stress Approach

Upcoming Challenges

- integration into flow solver for density ratios $\neq 1$
  - integral conservation law
  - sharp interface
  - conservative finite volume discretization
  - cut Cartesian grid cells
  - continuous approach

- reducing/minimizing spurious currents
  - due to pressure - surface force balance
  - due to large density ration between the two fluids

- 3D
Sharp Balanced Surface Stress Approach

Conservative Well-Balanced Sharp Interface Approach, 2D

momentum balance:

\[
\frac{d}{dt} \int_{\Omega} \rho u \, dV = - \int_{\partial \Omega} p^{(2)} n \, dS + \int_{\partial \Omega \cap \Gamma(t)} \sigma t \, dl
\]

aim: local second order scheme which handles interfaces forces well balanced AND conservative

idea: re-interpretation of the phase wise pressure data with pressure jump as continuous pressure jump field at old time level

\[
\int_{\partial \Omega} \sigma t \delta \Gamma \, dA = \int_{\partial \Omega \cap \partial \Gamma} \sigma t \, ds = \sigma_0 \int_{s_B} \kappa \tilde{n} \Gamma \, ds = \int_{\Omega \cap \partial \Gamma} [p] \, dA
\]
predictor

- pressure gradient term:
  - exact space-time integration of double bilinear pressure pressure ansatz functions on cell faces
  - movement of the levelset with possible change of curvature → geometrical usage of information on curvature change
  - neglect the impact of curvature change on pressure data (old time pressure data (implicitly gives $\llbracket p \rrbracket = \sigma \kappa$))
  - local extrapolation of pressure data for newly cut cells (care for symmetry) – naturally forces of opposed extrapolation in corrector step
Sharp Balanced Surface Stress Approach

Conservative Well-Balanced Sharp Interface Approach, 2D - dynamic case

**predictor**

- **surface force term:**
  - projection of surface force on cell faces (neglect bilinear information)
  - integration of temporally changed normal forces
    - consider temporal change of interface normal as change of projection on cell face
    - usage of old time pressure data on temporal changing interface (analogous to pressure gradient term handling)
  - pitfall: artificial time level breaks well balancing (earlier separation of two types of in-cell interface movement)

remark: No usage of explicit curvature data in predictor step! → fitting procedure instead of finite difference approximation in corrector step
Sharp Balanced Surface Stress Approach

projection of surface force term – usage of ONE machinery

\[
\int_{t_0}^{t_1} \int_{x_{j-1/2}}^{x_{j+1/2}} \mathbf{n}_y \, dl \, dt = \int_{t_0}^{t_1} \left[ \int_{x_0}^{x_{j+1/2}} [p] \, dx - \int_{x_0}^{x_{j-1/2}} [p] \, dx \right] \, dt
\]
Sharp Balanced Surface Stress Approach
Proof of concept for arbitrary and under-resolved cases – dynamic case (1)
Sharp Balanced Surface Stress Approach

Proof of concept for arbitrary and under-resolved cases – dynamic case (2)
Sharp Balanced Surface Stress Approach

Cut-cell Poisson extension / Implementation of space-time integration

- using of midpoint rule for spatial integration
- mid point value and interval length as linear time functions

\[
\int_{x_1}^{x_2} \int_{t_1}^{t_2} \nabla p(x, t) \, dt \, dx \approx \int \nabla p_m(t) \Delta x(t) \, t \, dt
\]

two opportunities: either difference of old time / new time curvature data as jump cond. OR old time pressure space time integral on rhs and new time curvature data as jump
Summary - well balance scheme

- **Currently:**
  - loc. sec. order scheme for a well balanced and conservative surface force handling (predictor)
  - loc. sec. order scheme for time dep. cut cell solver

- **Upcoming:**
  - frictionless case for soap bubble oscillations
    - usage of extrapolated pressure node / inexact levelsets
    - splitting of correction fluxes for velocity corrections
    - incremental vs. total corrector comparison
    - tangential force handling (dynamic)
    - investigation of damping behavior of the scheme
  - finally: case with friction and coefficient jumps (density etc.)