Energy preserving multiphase flows: Application to falling films.

N. Valle*, F.X. Trias and J. Castro

Universitat Politècnica de Catalunya - BarcelonaTech (UPC)

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Advantages

• Short residence time



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- Small temperature difference

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Applications

• Chemical industry



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Challenges

• Extreme density ratio



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- Short residence time
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- Chemical industry
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Challenges

- Extreme density ratio
- Hydrodynamic instability at Re = 0

Incompressible

$\nabla \cdot \vec{u} = 0$

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Interface

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$$\frac{\partial\theta}{\partial t} + \nabla \cdot (\vec{u}\theta) = 0$$

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$$rac{\partial heta}{\partial t} +
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Navier-Stokes

$$3Re\left(\frac{\partial\left(\rho\vec{u}\right)}{\partial t}+\nabla\cdot\left(\rho\vec{u}\otimes\vec{u}\right)\right)=\nabla\cdot\sigma+\rho\hat{g}$$

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$$\sigma = \mu S - p$$

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 $\sigma = \mu S - p \qquad \qquad [\sigma] \,\hat{\eta}_i = - W e \kappa \hat{\eta}_i$

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$$\theta = \frac{1}{2} \left(\tanh\left(\frac{d(\vec{x}}{2\epsilon} - 1\right) + 1\right)$$

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Regularization

$$heta = rac{1}{2} \left({ anh} \left(rac{{ extsf{d}}(ec{ extsf{x}}}{2\epsilon} - 1
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$$\rho = 1 + \left(\frac{\rho_1}{\rho_0} - 1\right)\theta$$

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$$E_m = E_k$$



$$E_m = E_k + E_p$$





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Discrete

Conservative Level-Set

$$\frac{d\theta_{\rm c}}{dt} = {\rm C}({\rm u}_{\rm f})_{\rm f}\theta_{\rm c}$$

Navier-Stokes - Continuum Surface Force¹

$$\frac{dHu_{\rm f}}{dt} = -C({\rm Ru}_{\rm f})_{\rm f}u_{\rm f} - {\rm Gp}_{\rm c} + {\rm Lu}_{\rm f} + Wek_{\rm f}{\rm G}\theta_{\rm c} + \rho_{\rm f}\hat{g}$$

¹ J.U Brackbill, D.B Kothe, and C Zemach. "A continuum method for modeling surface tension". In: J. Comput. Phys. 100.2 (June 1992), pp. 335–354.

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Performing a discrete energy balance:

$$\begin{aligned} \frac{dE_k}{dt} &= -\left(\mathsf{u}_{\mathsf{f}},\mathsf{C}(\mathsf{R}\mathsf{u}_{\mathsf{f}})_{\mathsf{f}}\mathsf{u}_{\mathsf{f}}\right) - \left(\mathsf{u}_{\mathsf{f}},\mathsf{G}\mathsf{p}_{\mathsf{c}}\right) + \left(\mathsf{u}_{\mathsf{f}},\mathsf{L}\mathsf{u}_{\mathsf{f}}\right) \\ &+ \mathit{We}\left(\mathsf{u}_{\mathsf{f}},\mathsf{k}_{\mathsf{f}}\mathsf{G}\theta_{\mathsf{c}}\right) + \left(\mathsf{u}_{\mathsf{f}},\rho_{\mathsf{f}}\hat{g}\right) \\ &- \frac{1}{2}\left(\mathsf{u}_{\mathsf{f}},\mathsf{u}_{\mathsf{f}}\Pi\frac{d\rho_{\mathsf{c}}}{dt}\right) \end{aligned}$$

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Discrete energy balance

Performing a discrete energy balance:

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$$\frac{dE_k}{dt} = -(u_f, C(Ru_f)_f u_f) - (\underline{u}_{f\tau}Gp_c) + (u_f, Lu_f) + We(u_f, k_fG\theta_c) + (u_f, \rho_f \hat{g}) - \frac{1}{2}(u_f, u_f\Pi \frac{d\rho_c}{dt})$$
$$\frac{dE_p}{dt} = We(GC(u_f)_c\theta_c, \hat{n}_f) - (u_f, \rho_f \hat{g})$$

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$$\begin{aligned} \frac{dE_k}{dt} &= -\left(\mathbf{u}_{f}, \mathsf{C}(\mathsf{Ru}_{f})_{f}\mathbf{u}_{f}\right) - \underbrace{\left(\mathbf{u}_{f\tau}\mathsf{G}\boldsymbol{p}_{c}\right)}_{\mathbf{h}} + \left(\mathbf{u}_{f}, \mathsf{Lu}_{f}\right) \\ &+ We\left(\mathbf{u}_{f}, \mathsf{k}_{f}\mathsf{G}\boldsymbol{\theta}_{c}\right) + \left(\mathbf{u}_{f}, \rho_{f}\hat{g}\right) \\ &- \frac{1}{2}\left(\mathsf{u}_{f}, \mathsf{u}_{f}\Pi\frac{d\rho_{c}}{dt}\right) \\ \frac{dE_{\rho}}{dt} &= We\left(\mathsf{GC}(\mathsf{u}_{f})_{c}\boldsymbol{\theta}_{c}, \hat{\mathsf{n}}_{f}\right) - \left(\mathsf{u}_{f}, \rho_{f}\hat{g}\right) \end{aligned}$$

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²N. Valle, F. X. Trias, and J. Castro. "An energy-preserving level set method for multiphase flows". In: J. Comput. Phys. 400 (2020), p. 108991. arXiv: 1909.01114.

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$$\frac{dE_m}{dt} = -\left(\mathbf{u}_{f}, \mathsf{C}(\mathsf{R}\mathbf{u}_{f})_{f}\mathbf{u}_{f}\right) + \left(\mathbf{u}_{f}, \mathsf{L}\mathbf{u}_{f}\right) - \frac{1}{2}\left(\mathbf{u}_{f}, \mathsf{U}\Pi\frac{d\rho_{c}}{dt}\right)$$

³Shahab Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096.

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$$= -\left(u_f, \frac{1}{2}diag\left(\Pi DRu_f\right)u_f\right)$$

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$$\begin{aligned} \frac{dE_m}{dt} &= -\left(\mathbf{u}_{f}, \mathsf{C}(\mathsf{R}\mathbf{u}_{f})_{f}\mathbf{u}_{f}\right) + \left(\mathbf{u}_{f}, \mathsf{L}\mathbf{u}_{f}\right) - \frac{1}{2}\left(\mathbf{u}_{f}, \mathsf{U}\Pi\frac{d\rho_{c}}{dt}\right) \\ &= -\left(\mathbf{u}_{f}, \frac{1}{2}\mathsf{U}\Pi\mathsf{D}\mathsf{R}\mathbf{u}_{f}\right) \end{aligned}$$

³Shahab Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096.

$$\begin{aligned} \frac{dE_m}{dt} &= -\left(\mathbf{u}_{f}, \mathsf{C}(\mathsf{R}\mathsf{u}_{f})_{f}\mathsf{u}_{f}\right) + \left(\mathbf{u}_{f}, \mathsf{L}\mathsf{u}_{f}\right) - \frac{1}{2}\left(\mathsf{u}_{f}, \mathsf{U}\Pi\frac{d\rho_{c}}{dt}\right) \\ &= -\left(\mathsf{u}_{f}, \frac{1}{2}\mathsf{U}\Pi\mathsf{D}\mathsf{R}\mathsf{u}_{f}\right) - \left(\mathsf{u}_{f}, \overline{\mathsf{C}(\mathsf{R}\mathsf{u}_{f})}\mathsf{u}_{f}\right) \end{aligned}$$

³Shahab Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096.

$$\frac{dE_m}{dt} = -\left(u_f, C(Ru_f)_f u_f\right) + \left(u_f, Lu_f\right) - \frac{1}{2}\left(u_f, U\Pi \frac{d\rho_c}{dt}\right)$$
$$= -\left(u_f, \frac{1}{2}U\Pi DRu_f\right) - \left(u_f, \overline{C(Ru_f)}u_f\right)$$

³Shahab Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096. ← □ → ← ⑦ → ← 毫 → ← 毫 → ← ₹ →

$$\begin{aligned} \frac{dE_m}{dt} &= -\left(u_f, C(Ru_f)_f u_f\right) + \left(u_f, Lu_f\right) - \frac{1}{2}\left(u_f, U\Pi \frac{d\rho_c}{dt}\right) \\ &= -\left(u_f, \frac{1}{2}U\Pi DRu_f\right) - \left(u_f, \overline{C(Ru_f)}u_f\right) \\ &+ \left(u_f, Lu_f\right) - \frac{1}{2}\left(u_f, U\Pi \frac{d\rho_c}{dt}\right) \end{aligned}$$

³Shahab Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096.

$$\begin{split} \frac{dE_m}{dt} &= -\left(u_f, \mathsf{C}(\mathsf{R}u_f)_f u_f\right) + \left(u_f, \mathsf{L}u_f\right) - \frac{1}{2}\left(u_f, \mathsf{U}\Pi \frac{d\rho_c}{dt}\right) \\ &= -\left(u_f, \frac{1}{2}\mathsf{U}\Pi\mathsf{D}\mathsf{R}u_f\right) - \left(u_f, \overline{\mathsf{C}(\mathsf{R}u_f)}u_f\right) \\ &+ \left(u_f, \mathsf{L}u_f\right) - \frac{1}{2}\left(u_f, \mathsf{U}\Pi \frac{d\rho_c}{dt}\right) \\ &\frac{d\rho_c}{dt} = \mathsf{C}(u_f)_f \rho_c = \mathsf{D}\mathsf{R}u_f \end{split}$$

³Shahab Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096. ← □ → ← ⑦ → ← 毫 → ← 毫 → ← ₹ →

$$\begin{aligned} \frac{dE_m}{dt} &= -\left(u_f, C(Ru_f)_f u_f\right) + \left(u_f, Lu_f\right) - \frac{1}{2} \left(u_f, U\Pi \frac{d\rho_c}{dt}\right) \\ &= -\left(u_f, \frac{1}{2} U\Pi DRu_f\right) - \left(u_f, \overline{C(Ru_f)} u_f\right) \\ &+ \left(u_f, Lu_f\right) - \frac{1}{2} \left(u_f, U\Pi \frac{d\rho_c}{dt}\right) \\ &\frac{d\rho_c}{dt} = C(u_f)_f \rho_c = DRu_f \end{aligned}$$

³Shahab Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096.

$$\begin{aligned} \frac{dE_m}{dt} &= -\left(u_f, C(Ru_f)_f u_f\right) + \left(u_f, Lu_f\right) - \frac{1}{2}\left(u_f, U\Pi \frac{d\rho_c}{dt}\right) \\ &= -\left(u_f, \frac{1}{2}U\Pi DRu_f\right) - \left(u_f, \overline{C(Ru_f)}u_f\right) \\ &+ \left(u_f, Lu_f\right) - \frac{1}{2}\left(u_f, U\Pi DRu_f\right) \\ &\frac{d\rho_c}{dt} = C(u_f)_f \rho_c = DRu_f \end{aligned}$$

 $^3 Shahab$ Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096.

$$\begin{aligned} \frac{dE_m}{dt} &= -\left(u_f, \mathsf{C}(\mathsf{Ru}_f)_f u_f\right) + \left(u_f, \mathsf{Lu}_f\right) - \frac{1}{2}\left(u_f, \mathsf{U}\Pi \frac{d\rho_c}{dt}\right) \\ &= -\left(u_f, \frac{1}{2}\mathsf{U}\Pi\mathsf{D}\mathsf{Ru}_f\right) - \left(u_f, \overline{\mathsf{C}(\mathsf{Ru}_f)} u_f\right) \\ &+ \left(u_f, \mathsf{Lu}_f\right) - \frac{1}{2}\left(u_f, \mathsf{U}\Pi\mathsf{D}\mathsf{Ru}_f\right) \\ &\frac{d\rho_c}{dt} = \mathsf{C}(u_f)_f \rho_c = \mathsf{D}\mathsf{Ru}_f \end{aligned}$$

Energy-preserving discretization

$$\frac{dE_m}{dt} = (u_f, Lu_f) < 0$$

³Shahab Mirjalili and Ali Mani. "Consistent, energy-conserving momentum transport for simulations of two-phase flows using the phase field equations". In: *J. Comput. Phys.* 1 (2020), p. 109918. arXiv: 1912.10096.

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Falling Film



Falling Film




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Figure: Energy fluctuation for the falling film

Simulation of industrial falling films

id	fluid	$T(^{\circ}C)$	X_{abs}	Ka	$\Pi_ ho(imes 10^{-3})$	$\Pi_{\mu}(imes 10^{-3})$
Α	H_2O	9.9	0.00	2420	0.60	9.37
В	H ₂ O/LiBr	50.0	0.60	443	0.35	2.45
С	H ₂ O/Carrol	50.0	0.67	150	0.35	1.10

Table: Estimated fluid properties dimensionless groups. Because thermal properties are estimated at a characteristic state, values are rounded to ease its handling.

DNS of vertically falling films



Figure: Velocity magnitude on the film surfaces for cases A, B and C at Re = 150 after T = 100.



• Consistent mass and momentum transfer





- Consistent mass and momentum transfer
- Energy-preserving discretization

Summary

- Consistent mass and momentum transfer
- Energy-preserving discretization
- Enhanced stability

Summary

- Consistent mass and momentum transfer
- Energy-preserving discretization
- Enhanced stability
- Physical reliability