Direct numerical simulation of interfacial instability in gas-liquid flows

Iain Bethune¹, Lennon Ó Náraigh^{* 2}, David Scott¹, Peter Spelt^{3,4}, Prashant Valluri⁵, Zlatko Solomenko³

 ¹Edinburgh Parallel Computing Centre, University of Edinburgh, James Clerk Maxwell Building, Mayfield Road, Edinburgh EH9 3JZ, UK
 ²School of Mathematics and Statistics, University College Dublin, Ireland
 ³Département Mécanique, Université de Lyon 1
 ⁴Laboratoire de Mécanique des Fluides et dAcoustique (LMFA), CNRS, Ecole Centrale de Lyon, 69134 Ecully, France
 ⁵Institute of Materials and Processes, Sanderson Building, School of Engineering, University of Edinburgh, Kings Buildings, Edinburgh EH9 3JL, UK

15th May 2017

Context

Two-phase stratified flow is ubiquitous in nature.



- Mathematically, and computationally, a tough problem turbulence, extreme nonlinearity, topological change in interfaces, a range of instabilities that need to be captured.
- Even the laminar regime is tough current focus of the research.

Context: The numerical challenge

- Flows involving many length- and time-scales
- Flows with sharp changes in interfacial topologies
- Transient three-dimensional simulations required over long periods of time, requiring scalable codes run at very high resolutions.



• Existing interface-capturing methods: Levelset, Volume of Fluid, Particles, Diffuse Interface Method

- Existing interface-capturing methods: Levelset, Volume of Fluid, Particles, Diffuse Interface Method
- Existing implementations: Open-source (e.g. Gerris, etc.), Commercial (CFX, etc.), in-house solvers.

- Existing interface-capturing methods: Levelset, Volume of Fluid, Particles, Diffuse Interface Method
- Existing implementations: Open-source (e.g. Gerris, etc.), Commercial (CFX, etc.), in-house solvers.
- Some drawbacks (not respectively): Black-box approach, validation uncertain, artificial diffusion. Key drawbacks: resolution constraints, scalability.

- Existing interface-capturing methods: Levelset, Volume of Fluid, Particles, Diffuse Interface Method
- Existing implementations: Open-source (e.g. Gerris, etc.), Commercial (CFX, etc.), in-house solvers.
- Some drawbacks (not respectively): Black-box approach, validation uncertain, artificial diffusion. Key drawbacks: resolution constraints, scalability.
- Our in-house code **TPLS** addresses these issues, in particular **resolution and scalability**.

- Existing interface-capturing methods: Levelset, Volume of Fluid, Particles, Diffuse Interface Method
- Existing implementations: Open-source (e.g. Gerris, etc.), Commercial (CFX, etc.), in-house solvers.
- Some drawbacks (not respectively): Black-box approach, validation uncertain, artificial diffusion. Key drawbacks: resolution constraints, scalability.
- Our in-house code **TPLS** addresses these issues, in particular **resolution and scalability**.
- Not a silver bullet levelset methods tradeoff between capturing interfacial topology with great fidelity, and mass loss. But mass loss minimized at high resolution.

TPLS: Equations of motion

Numerical solution of two-phase Navier-Stokes equations with interface capturing:

$$\rho(\phi) \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot \left[\mu(\phi) \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T \right) \right] + \boldsymbol{f}_{\text{st}}(\phi) - \rho(\phi) \mathcal{G} \hat{\boldsymbol{z}},$$

where $\nabla\cdot\mathbf{u}=0$ and ϕ is the interface-capturing field:

TPLS: Equations of motion

Numerical solution of two-phase Navier-Stokes equations with interface capturing:

$$\rho(\phi) \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot \left[\mu(\phi) \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T \right) \right] + \boldsymbol{f}_{\text{st}}(\phi) - \rho(\phi) \mathcal{G} \hat{\boldsymbol{z}},$$

where $\nabla\cdot\mathbf{u}=0$ and ϕ is the interface-capturing field:

Levelset method:

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0, \qquad \boldsymbol{f}_{\rm st} = \delta_{\epsilon}(\phi) \frac{1}{\rm We} \boldsymbol{\widehat{n}} \nabla \cdot \boldsymbol{\widehat{n}}. \qquad \boldsymbol{\widehat{n}} = \frac{\nabla \phi}{|\nabla \phi|}.$$

TPLS: Equations of motion

Numerical solution of two-phase Navier-Stokes equations with interface capturing:

$$\rho(\phi) \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot \left[\mu(\phi) \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T \right) \right] + \boldsymbol{f}_{\text{st}}(\phi) - \rho(\phi) \mathcal{G} \hat{\boldsymbol{z}},$$

where $\nabla\cdot\mathbf{u}=0$ and ϕ is the interface-capturing field:

Levelset method:

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0, \qquad \boldsymbol{f}_{\rm st} = \delta_{\epsilon}(\phi) \frac{1}{\rm We} \boldsymbol{\widehat{n}} \nabla \cdot \boldsymbol{\widehat{n}}. \qquad \boldsymbol{\widehat{n}} = \frac{\nabla \phi}{|\nabla \phi|}.$$

Dimensionless groups:

$$Re = \frac{\rho_T V L}{\mu_T}, \qquad \mathcal{G} = \frac{gL}{V^2}, \qquad We = \frac{\rho_T L V^2}{\gamma},$$
(I also use $\mathcal{S} = 1/We$, for historical reasons!)

TPLS: Problem geometry and configuration

- Simple channel geometry: periodic boundary conditions at x = 0, $x = L_x$; walls (no slip) at z = 0, $z = L_z$.
- Constant pressure drop drives flow in streamwise direction (forcing).
- Basic version involves hydrodynamics only. TPLS with physics under development, for applications including contact-line dynamics, and mass transfer.



• Marker-and-cell discretization: pressures, densities, viscosities, and ϕ at cell centres, velocities at cell faces.

- Marker-and-cell discretization: pressures, densities, viscosities, and ϕ at cell centres, velocities at cell faces.
- Finite-volumes, with flux-conservative differencing for the momentum equation.

- Marker-and-cell discretization: pressures, densities, viscosities, and ϕ at cell centres, velocities at cell faces.
- Finite-volumes, with flux-conservative differencing for the momentum equation.
- Momentum step: centred differences for the convective derivative, Crank–Nicholson treatment for the diffusion, third-order Adams–Bashforth for the time evolution.

- Marker-and-cell discretization: pressures, densities, viscosities, and ϕ at cell centres, velocities at cell faces.
- Finite-volumes, with flux-conservative differencing for the momentum equation.
- Momentum step: centred differences for the convective derivative, Crank–Nicholson treatment for the diffusion, third-order Adams–Bashforth for the time evolution.
- Projection method: Momenta are updated first, followed by a correction step involving a pressure update, thereby enforcing incompressibility.

- Marker-and-cell discretization: pressures, densities, viscosities, and ϕ at cell centres, velocities at cell faces.
- Finite-volumes, with flux-conservative differencing for the momentum equation.
- Momentum step: centred differences for the convective derivative, Crank–Nicholson treatment for the diffusion, third-order Adams–Bashforth for the time evolution.
- Projection method: Momenta are updated first, followed by a correction step involving a pressure update, thereby enforcing incompressibility.
- The levelset function $\phi(x, y, z, t)$ is carried with the flow (3rd-order WENO) but is corrected at each timestep ('redistancing').

• Typical runs involve up to 10 million gridpoints, meaning that large-scale parallel simulation is unavoidable (larger runs (up to 100 million gridpoints) are also performed).

- Typical runs involve up to 10 million gridpoints, meaning that large-scale parallel simulation is unavoidable (larger runs (up to 100 million gridpoints) are also performed).
- Code is parallelized using hybrid MPI technology; parallelization scheme takes account of problem geometry (2D domain decomposition)

- Typical runs involve up to 10 million gridpoints, meaning that large-scale parallel simulation is unavoidable (larger runs (up to 100 million gridpoints) are also performed).
- Code is parallelized using hybrid MPI technology; parallelization scheme takes account of problem geometry (2D domain decomposition)
- Data is outputted to files periodically using parallel I/O NetCDF data storage.
- Current version of code with density contrast uses simple hand-coded algorithms for linear algebra steps (e.g. presuse step). Work is ongoing to replace these with GMRES by repeated calls to the PETSc library.

- Typical runs involve up to 10 million gridpoints, meaning that large-scale parallel simulation is unavoidable (larger runs (up to 100 million gridpoints) are also performed).
- Code is parallelized using hybrid MPI technology; parallelization scheme takes account of problem geometry (2D domain decomposition)
- Data is outputted to files periodically using parallel I/O NetCDF data storage.
- Current version of code with density contrast uses simple hand-coded algorithms for linear algebra steps (e.g. presuse step). Work is ongoing to replace these with GMRES by repeated calls to the PETSc library.

- Typical runs involve up to 10 million gridpoints, meaning that large-scale parallel simulation is unavoidable (larger runs (up to 100 million gridpoints) are also performed).
- Code is parallelized using hybrid MPI technology; parallelization scheme takes account of problem geometry (2D domain decomposition)
- Data is outputted to files periodically using parallel I/O NetCDF data storage.
- Current version of code with density contrast uses simple hand-coded algorithms for linear algebra steps (e.g. presuse step). Work is ongoing to replace these with GMRES by repeated calls to the PETSc library.
- Parallel efficiency with 2000 MPI processes is only 0.6 there is a tradeoff between robustness/simplicity and performance. Underscores the need to replace hand-coded linear-algebra solvers with libraries.

Strict benchmarks for code's accuracy

- Introduce a tiny sinusoidal perturbation at the interface.
- Produces pressure and velocity fluctuations that satisfy linear equations of motion.
- Linearized equations of motion solved via eigenvalue analysis (independent, quasi-analytical).
- Gives growth rate and wave speed of wave-like fluctuations.



Focus on finding agreement between OS analysis and wave growth in the code.

Orr-Sommerfeld analysis - Results



Application of TPLS: where do 3D waves in parallel flows come from?



Linear instability of 2D parallel flow is dominated by 2D waves. So how do 3D structures form?



Brief review for liquid-liquid flows

We know the answer for liquid-liquid flows (r = 1) – it is weakly nonlinear analysis.

Streamwise waves - Large temporal growth, Spanwise waves - No temporal growth rate



 Streamwise overtones are enslaved to the streamwise dominant mode Purely spanwise mode enslaved to the dominant streamwise mode

Periodic boundary conditions, (Re, m, r, S) = (300, 30, 1, 0.3).

New study required for gas-liquid flows

For gas-liquid flows, linear theory predicts a direct route.



(a) r = 100, S = 0.1 (b) r = 1000, S = 0.1

Eigenvalue analysis of the two-phase Orr–Sommerfeld–Squire equations for $Re = 100, m = 30, h_0 = 0.3$, and $\mathcal{S} = 0.1$, and $\mathcal{G} = 0.1$.

New study required for gas-liquid flows

For gas-liquid flows, linear theory predicts a direct route.



(a) r = 100, S = 0.1 (b) r = 1000, S = 0.1

Eigenvalue analysis of the two-phase Orr–Sommerfeld–Squire equations for $Re = 100, m = 30, h_0 = 0.3$, and $\mathcal{S} = 0.1$, and $\mathcal{G} = 0.1$.

Overall trend: increasing r means that more modes become unstable (both streamwise and spanwise), but with a smaller growth rate.

Theoretical Prediction confirmed by DNS



DNS results (lines with circles) for the case ($m = 50, h_0 = 0.2, \mathcal{G} = 0.1, We = 10$), with r = 1000 and Re = 500. Shown also is a comparison with linearized DNS (unadorned lines). Here, $\alpha_0 = 2\pi/L_x$ and $\beta_0 = 2\pi/L_y$ denote the fundamental wavenumber in the streamwise and spanwise directions respectively. In panel (c) the growth of the relevant amplitude is modest and a vertical linear (as opposed to logarithmic) scale is used. Also, the 'kink' at t = 2 in the same panel simply corresponds to a zero of $\xi_{0\beta_0}(t)$, as this particular Fourier amplitude does not grow exponentially.

2D-DNS used to construct a flow-pattern map



Flow-pattern map for the two-dimensional simulations. The non-dimensionalization is based on the upper-layer properties, with $(m = 50, h_0 = 0.2, \mathcal{G} = 0.1, We = 10)$. Squares – Dispersed liquid phase. Circles – ligaments. Triangle – saturated travelling wave. The insets show snapshots of the three different flow regimes.

Carefully-chosen 3D simulations show the results carry over



DNS results for the case $(m = 50, h_0 = 0.2, \mathcal{G} = 0.1, We = 10)$, with r = 1 and Re = 500.

The case r = 10



FIG. 30. DNS results for the case $(m = 50, h_0 = 0.2, \mathcal{G} = 0.1, We = 10)$, with r = 10 and Re = 500.

The case r = 100



DNS results for the case $(m = 50, h_0 = 0.2, \mathcal{G} = 0.1, We = 10)$, with r = 100 and Re = 500.

• TPLS has been introduced as a computational methodology for two-phase simulations in an idealized channel geometry.

- TPLS has been introduced as a computational methodology for two-phase simulations in an idealized channel geometry.
- Using TPLS, we answer the question, where do 3D waves in parallel flows come from?

- TPLS has been introduced as a computational methodology for two-phase simulations in an idealized channel geometry.
- Using TPLS, we answer the question, where do 3D waves in parallel flows come from?
- For liquid-liquid flows an indirect (weakly nonlinear) mechanism prevails.

- TPLS has been introduced as a computational methodology for two-phase simulations in an idealized channel geometry.
- Using TPLS, we answer the question, where do 3D waves in parallel flows come from?
- For liquid-liquid flows an indirect (weakly nonlinear) mechanism prevails.
- Using theory and DNS, our current work shows a different scenario at work in gas-liquid flows:
 - The interfacial waves in gas-liquid ows grow much more slowly than those in corresponding liquid-liquid flows.
 - However, a wider range of wavenumbers (both streamwise and spanwise) are unstable for the gas-liquid case.

- TPLS has been introduced as a computational methodology for two-phase simulations in an idealized channel geometry.
- Using TPLS, we answer the question, where do 3D waves in parallel flows come from?
- For liquid-liquid flows an indirect (weakly nonlinear) mechanism prevails.
- Using theory and DNS, our current work shows a different scenario at work in gas-liquid flows:
 - The interfacial waves in gas-liquid ows grow much more slowly than those in corresponding liquid-liquid flows.
 - However, a wider range of wavenumbers (both streamwise and spanwise) are unstable for the gas-liquid case.

Therefore, three-dimensional waves form in gas-liquid ows via a **direct route**: by waiting long enough, streamwise and spanwise modes form as a result of small-amplitude perturbations.

- TPLS has been introduced as a computational methodology for two-phase simulations in an idealized channel geometry.
- Using TPLS, we answer the question, where do 3D waves in parallel flows come from?
- For liquid-liquid flows an indirect (weakly nonlinear) mechanism prevails.
- Using theory and DNS, our current work shows a different scenario at work in gas-liquid flows:
 - The interfacial waves in gas-liquid ows grow much more slowly than those in corresponding liquid-liquid flows.
 - However, a wider range of wavenumbers (both streamwise and spanwise) are unstable for the gas-liquid case.

Therefore, three-dimensional waves form in gas-liquid ows via a **direct route**: by waiting long enough, streamwise and spanwise modes form as a result of small-amplitude perturbations.

• Beyond this early-stage wave growth, a zoo of dierent phenomena is possible, depending on the particular ow parameters involved.