Simulation numérique de l'atomisation

Stéphane Zaleski & Yue Ling

Institut Jean Le Rond d'Alembert, CNRS & Université Pierre et Marie Curie – UPMC – Paris 6

web site http://www.ida.upmc.fr/~zaleski







Typical structure and simulation strategy









Simulation methodology







VOF methodology







- I Compute an evolving surface : computational geometry
- Solve
 - 2 the Navier-Stokes equations with
 - 3 surface tension,

and

- 4 variable viscosity and density,
- 5 ensure robustness,
- 6 have a multiscale approach.









Old Codes:

Surfer Gerris gfs.sf.net

New codes

Basilisk basilisk.fr ParisSimulator parissimulator.sf.net

Improvements: better stability, accuracy, faster, HPC-compatible.

All our codes are free.







Gerris is very accurate: Capillary wave test. L_2 error norm:

Method/resolution	8	16	
Present study (Gerris)	0.1568	0.0279	
CLSVOF [66]	0.3169	0.0991	
CSF [19]	-	-	
RLSG [40]	-	0.1116	
Front-tracking [15]	0.3018	0.0778	









Atomization







Kelvin-Helmholtz instability : unstable shear flow









2D simulations of the planar « Grenoble » setup.

Gas Liquid

The Grenoble quasi 2D experiment set up







Use Gerris flow solver with adaptive oct-tree and quad-tree grids



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Elementary multiscale treatment: Navier-Stokes with variable minimum grid size according to a subdivision of the computational domain.







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Simulation with a separator plate at density ratio (1/r = 100)

т	r	Re_g	Re_l	We_{g}	We_l	M
0.017	0,01	2640	290	19	8	2,4



Movie by Daniel Fuster and Jérôme Hoepffner using the Gerris Flow solver









Compare to experiments in Grenoble (Cartellier, Matas) . Flow from right to left. Video with help of Jérôme Hoepffner and Jon Soundar.







To compare numerical results with theory, we need:

Linear stability theory of the Kelvin-Helmholtz instability: Viscous, Error-function profiles

- a) Yecko, Fullana, Boeck, Zaleski,
- b) Gordillo, Perez-Saborid, Ganan-Calvo,
- c) Spelt, Valluri, O'Naraigh
- d) Matas







Convective/absolute instabilities

I) Absolute: a spatially localized perturbation at x=0 and t=0 grows in the entire space



corresponds to a well-defined oscillator frequency in the entire domain, a so-called « global mode ». Upstream turbulence has little influence.







Convective/absolute instabilities

2) Convective instability: a spatially localized perturbation at t=0 is convected downstream with the flow



No single frequency is observed but instead, broadband noise is seen. The system is seen to be a noise amplifier. Upstream turbulence matters





So what does linear theory say about our problem ? Is it convective or absolute ?

Linear theory has an enormous dependence on the wake flow correction.





Simplified base flows







Effect of upstream turbulence on instability growth.

The effect of upstream turbulence will be important if the spatial analysis reveals a convective instability.

It will be unimportant if an absolute instability is found.







Most « important » parameter: momentum flux ratio (or ratio of dynamic pressures. It is the only parameter that does not involve small-scale characteristics of the flow)

$$M = \frac{\rho_g u_g^2}{\rho_l u_l^2}$$









Grenoble experiments: Cartellier, Matas, Marty

Now the ultimate test ! Compare :

- Experiments
- Numerics
- Linear theory

We need linear theory, again but for spatially developping flows.

For that, we need to know what are absolute and convective instabilities !







What about the simulation ?







Comparison experiment-simulation







3D flows







The iconic Marmottant-Villermaux case



Air-Water $u_{liq} = 0.6 \text{ m s}^{-1}, u_{gas} = 35 \text{ m s}^{-1}$

injection diameter D = 7.8 mm

 $Re_g = 16000, We_g = 200$ based on D₁

 $\operatorname{Re}_{\delta}$ = 400

Simulation : six weeks on 64 AMD processors

line of eight 512³ boxes – (equivalent regular mesh but we use octree adaptation)

Difficult to go to higher levels of refinement









Boundary layer size 157 µm

smallest grid size 50 µm

25µm case currently running

Injector thickness comparable.



















experimental and computed at UPMC

$$u_2 = 35 \text{ m} / \text{s}$$







Lagrangian Point Particle model







- Resolved Flow (Popinet, 2009) $\rho(\partial_t u + u \cdot \nabla u) = -\nabla p + \nabla \cdot (2\mu D) + \sigma \kappa \delta_s n - f_p$ $\nabla \cdot u = 0$ $\partial_t c + u \cdot \nabla c = 0$
- Lagrangian Point-Particle $du_{n} \quad \tilde{u} - u_{n} \quad \rho D\tilde{u} \quad C_{m}\rho (D\tilde{u} \quad du_{n})$

$$\frac{d\boldsymbol{u}_p}{dt} = \frac{\boldsymbol{u} - \boldsymbol{u}_p}{\tau_p} \phi + \frac{\rho}{\rho_p} \frac{D\boldsymbol{u}}{Dt} + \frac{C_m \rho}{\rho_p} \left(\frac{D\boldsymbol{u}}{Dt} - \frac{d\boldsymbol{u}_p}{dt}\right)$$







The modelling depends on the type of simulation.



With oct-treeAMR we will move from more or less resolved cases.

Do simultaneously VOF->LPP conversion and massive grid coarsening ?

Question: (unanswered) how much accuracy do we lose by going from a fully resolved drop to a « very unresolved » one

In a first step we work on a regular cubic grid code without AMR, ParisSimulator







Test case : driven cavity flow with LPP. Re=16, Re_p =0,34



Pulsed Diesel-type jet

























VOF to LPP conversion - Higher Reynolds



Conditions de l'article de Deschamp et al dans lequels les trajectoires de particules sont mesurées

 $\operatorname{Re}_{\delta}$ = 1000

Simulation $64 \times 256 \times 512$







Coflowing air and liquid jets (moderate density ratio)





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Simulation $128 \times 512 \times 1024$











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PDF of droplet diameters – (a) t = 0.4s, (b) t = 0.41s, and (c) t = 0.42s.







Immediate Perspectives:

- A well understood, consistent, verified theory of the 3D instability: at present many theories, and almost no numerics.

- A proof of convergence of the Lagrangian point particle model.

- VOF technology: AMR-VOF-LPP with basilisk. (new octree code).

Longer term perspectives:

- coupling with thermal / reaction effects.
- use DNS to develop and validate large-scale particle ejection models.
- full combustion chamber simulations.







Simulation methodology



Collaborators past and present.

Jie Li (Cambridge UK), Denis Gueyffier (ONERA Paris), Phil Yecko (Montclair, NJ), Thomas Boeck (Ilmenau), Jose-Maria Fullana (d'Alembert), Ruben Scardovelli (Bologna), Christophe Josserand (d'Alembert), Stéphane Popinet (d'Alembert), Pascal Ray (d'Alembert), Luis Lemoyne (Nevers), Shahriar Afkhami (NJIT), Gaurav Tomar (Bangalore), Daniel Fuster (d'Alembert), Anne Bagué, Jérôme Hoepffner (d'Alembert). Gilou Agbaglah (Michigan), J. John Soundar Jerome (Lyon), Arup K. Das (IITG).

Current Students and postdocs

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The End

ρι	100		
(Kg/m3)			
ρ _g	1		
(Kg/m3)			
μι	1.00E-03		
(Kg/s m)			
μ _g	1.00E-05		
(Kg/s m)			
dp	0.02		
(mm)			
U ₀	0.5		
	0.5		

