

FULL RESEARCH PROPOSAL APPLICATION RECEIPT RECORD

(FAST-START PROPOSAL)

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Fast-Start proposal	Application number: 01-NIW-021	Panel(s): PSE
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From: Administration Officer  
Marsden Fund  
The Royal Society of NZ  
PO Box 598  
WELLINGTON

# MARSDEN FUND FULL RESEARCH PROPOSAL (FAST-START)

## 1 IDENTIFICATION

### 1.1.1

#### 1.1.2 Principal Investigator

Name & Title:	Stéphane Popinet Dr
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## 2 TITLE OF RESEARCH PROPOSAL

Generic and accurate direct numerical simulation of interfacial and free-surface flows

### 3 3. SUMMARY

Describe in up to 200 words the nature of your proposed research in plain English for a general audience. This summary should be able to be used for publicity purposes if the proposal is offered funding.

Interfaces between fluids play a very important role in many physical processes in a variety of domains. Sea/atmosphere interaction through wave breaking, rain droplet formation in clouds, jet atomisation in internal combustion or rocket engines, fluid models for atomic fusion, fluid/structure coupling in offshore engineering and biomechanics are just a few examples where our current knowledge of interfacial dynamics is very limited. Numerical simulations can be a very powerful tool in performing the experiments needed for a better understanding of these processes. However, despite recent developments in numerical techniques for interface representation, none of the available methods combine accuracy in the treatment of surface terms and generality in the type of problems treated. In particular, many applications involving three-dimensional interfaces with large deformations and strong surface forces are still beyond the capabilities of current simulation tools. Small and medium scale air/water flows are a typical example. This project aims to fill this gap by simulating three-dimensional interfacial flows, introducing novel techniques for dealing accurately and efficiently with surface terms even in the case of large interface deformations. The project should also provide a generic simulation tool for three-dimensional interfacial flows.

#### 4.4. BACKGROUND

Using only this page, give a context for the proposal by summarising in plain English the state of knowledge in the field.

Numerical simulations of fluid flow have been among the first scientific applications of computing. While single-phase flow simulation tools are now widely used both for engineering (in particular in the aeronautical and automotive industries) and research purposes, multiphase flows with interfaces (e.g., gas bubbles in water) remain difficult to model [1,2]. The various available methods differ essentially in two ways: (i) representation of the hydrodynamic fields in each of the phases, (ii) coupling of the hydrodynamic fields with the interface representation and the associated boundary conditions (surface forces and discontinuities in physical properties).

In some cases, the representation of hydrodynamic fields can be greatly simplified. Boundary integral techniques [3,4] make the assumption of a potential flow, which reduces the problem to the computation of the distribution of vorticity sources located on the interface. While appealing for their clean mathematical formulation, these methods are only applicable to the asymptotic limits of very high or very low viscosity flows. In the general case it is necessary to represent the spatial structure of the flow, which is done through discretisation of the hydrodynamic variables on a computational grid. The type of grid used depends essentially on the way the coupling with the interfacial boundary conditions is performed.

It may seem preferable to use discrete elements which are entirely contained in one of the phases. The multiphase problem then reduces to single-phase problems linked by boundary conditions along the interface. Finite elements [5,6] or conformal mapping [7,8] techniques used for single-phase flows in complex geometrical domains can be adapted to solve these problems. The interface is a moving boundary condition and consequently a deformable grid is required. These moving grid techniques are appealing because of the straightforward and accurate representation of the interface and boundary conditions. However, in many applications the interface can undergo large deformations or even topology changes (e.g., reconnection and break up). Complete re-meshing of the computational domain is then necessary at regular intervals. This makes moving grid techniques computationally complex and expensive.

When a fixed grid is used, the interface can be represented either explicitly or implicitly. Implicit representations use a separate phase function discretised on the fixed grid which indicates which phase is present at a given location. The interface is then implicitly defined as the location of rapid phase function variation. Two classical implicit representations are the Volume Of Fluid (VOF) [9,10,11] technique, and the Level Set technique [12,13]. In implicit methods, interface motion is simply obtained by advection of the corresponding phase function. These techniques are computationally relatively simple and deal transparently with large interface deformations and topology changes [14,15].

Recently introduced, explicit interface representations rely on a separate mesh of lower dimension (curve in 2D and surface in 3D) which describes accurately the location and geometry of the interface [16,17,18]. The mesh is transported and deformed by the flow and some form of re-meshing is then necessary.

Fixed grid methods must ensure that boundary conditions on the interface are verified. This is particularly important in the case of strong surface forces like surface tension. When using an implicit representation it is difficult to obtain accurate values for the geometrical properties of the interface (such as curvature) necessary for the computation of boundary conditions. These methods thus generally rely on some form of averaging which spreads surface terms over a few computational cells resulting in a numerically thick interface [11,19]. The accuracy of the resulting solution is questionable and in many regimes of practical interest (e.g., high surface tension and low viscosity typical of air/water flows) inconsistencies in the computation of surface tension forces and pressure gradient may

prevent any simulation [2,14,20]. On the other hand, explicit representations, while computationally more complex allow direct access to geometrical properties and have been shown to yield accurate solutions even in the case of large interface deformations and strong surface forces [20,21,22,23].

## 5 5. OVERALL AIM OF THE RESEARCH

Using only this page, state the general goals and specific objectives of the research proposal. Emphasise how the research will advance knowledge and increase understanding.

The overall aim of the proposed research is to extend and generalise our 2D front-tracking technique [20,21] to three dimensions. The method relies on a fixed grid discretisation of the hydrodynamic fields and uses an explicit representation of the interface through a separate mesh.

The primary objective is to provide a treatment of surface terms comparable in accuracy to moving grid techniques while allowing large interface deformations at a relatively low computational cost. This will allow the numerical simulation of many regimes of practical interest which are difficult or impossible to model using current simulation techniques.

The extension to three dimensions will be done through a systematic use of a finite volume approach treating the interface as a real boundary between discrete elements.

The objective here is to provide a mathematically correct formulation of surface terms as well as a physically correct treatment of the interface as a real discontinuity, in contrast to the currently available fixed grid methods.

This approach is also intended to lead to a generic framework which will allow easy implementation of a variety of boundary conditions (e.g., varying surface tension, free-surfaces, solid boundaries, elastic membranes), thus opening a large field of applications.

The extraction of finite volumes in the vicinity of the interface will rely on set operations (intersection, difference) between 3D surfaces.

To achieve this we need to develop robust numerical evaluation tools for such operations. This approach has a large number of applications in different fields (e.g., computational geometry, computer aided design or computer graphics). Starting from our preliminary work [24], this project will provide reusable and documented functions (libraries) to perform these operations as well as others (surface mesh simplification and refinement in particular).

The whole project will rely on an open development model: other researchers will be provided with easy access to source code in order to increase international cooperation and feedback.

## 6.6. PROPOSED RESEARCH

This section should cover where appropriate the hypotheses being tested, the methodology to be used, sampling design, and methods of data analysis. Indicate the intended research programmes of all researchers including postdoctoral fellows or postgraduate students, if any. FTE requests need to be justified. Please use a MAXIMUM of 3 pages.

The development of a front-tracking algorithm poses two main problems:

1. A kinematic problem: Lagrangian transport and deformation of the chosen representation of the interface.
2. A dynamical problem: coupling of the interface representation with the underlying discretisation used to solve the equations of motion.

We have chosen to represent the interface as a separate mesh of triangular elements. These elements are defined through the Cartesian coordinates of their vertices and their neighbourhood relationships. The kinematic problem is then largely independent of the discretisation used to solve the equations of motion. We only need to define an interpolation function which will return the velocity of a given vertex. At each time step, the coordinates of the vertices are updated according to the interpolated velocity.

As the shape and size of the interface evolves, it is necessary to ensure that the quality of the mesh is preserved. For example, if the interface is stretched by the flow, it may be necessary to increase locally the number of triangular elements and conversely in the areas which are contracted by the flow. It makes sense to ensure that the local discretisation scale of the interface (i.e., the size of a triangular element) is always comparable to the discretisation scale of the underlying hydrodynamic grid. Other quality criteria can also be investigated (curvature-based or error-based in particular).

These local mesh refinement or coarsening procedures are similar to techniques used in computer graphics [25,26,27,28]. It is also important to conserve the total volume of the interface while performing these operations. The techniques we have already implemented in the GTS library [24,28] are well suited but will need to be adapted and tested for this particular case.

The dynamical problem will certainly prove more challenging and we consequently propose to start with a simplified implementation which will help identify and solve potential problems. We will thus limit the initial simulations to incompressible two-phase flows of fluids of identical physical properties (density and viscosity) but with surface tension. A classical projection method [29] will be used on a regular 3D Cartesian grid to solve the incompressible Navier-Stokes equations [14]. In the momentum control volumes (discretisation cells) cut by the interface, it will be necessary to compute the integral contribution of surface tension as a source term in the momentum equation. We propose to do that by integrating numerically the surface tension term (a function of the local curvature and normal to the interface) along the piece of interface contained in a given control volume. These pieces of interfaces will be obtained through Boolean operations (intersection) between the interface mesh and the control volumes (cubes in the case of a Cartesian mesh).

In a spirit similar to the pressure-gradient correction approach presented in [20], we will deal precisely with the pressure jump (due to surface tension) occurring at the interface. We anticipate that this will only require the computation of surface fractions (fraction of the side of a given cell occupied by one of the fluid) in the control volumes cut by the interface. These will be obtained through the same Boolean operations used for the computation of the integral contribution of surface tension.

First validation tests will include the now classical case of a bubble in a stationary fluid with

surface tension at the interface. In that case, Laplace's law implies that surface tension is exactly balanced by the pressure jump across the interface. This has been shown not to be the case for most numerical methods using fixed grids (including VOF [14,11,20] and Level Set) with the presence of the so-called "spurious currents". In this 3D implementation, we should obtain the same second order convergence to the theoretical solution that we observed with the two dimensional code [20]. Other tests possible with this simplified preliminary version include plane capillary waves and modes of deformation of an initially spherical bubble.

The approach we propose requires an efficient and robust way to compute Boolean operations between discretised surfaces. This is a classical problem in the field of computational geometry [30] and computer graphics [31,32] and we have implemented a preliminary but already functional version as part of the GTS library. Robustness of geometrical algorithms is not straightforward due to the inconsistencies caused by round-off errors when performing simple operations such as orientation tests [33,34]. A number of solutions have been proposed in recent years [35] and robust geometric predicates [36] are used throughout the GTS library to avoid these problems. The 3D front-tracking algorithm will be a quite stringent test of the Boolean operations but we are confident that we will be able to make the improvements which may be necessary.

This preliminary version will help set up a generic formulation within which density and viscosity changes across the interface will be allowed. An integral formulation similar to the 2D-axisymmetric free-surface formulation presented in [21,37] will ensure an accurate discretisation of the terms which can be discontinuous across the interface, such as the viscous terms in the momentum equation. We expect that the implementation of this integral formulation will be largely simplified by the direct use of the Boolean operations to obtain the integration domains.

Potential tests of this complete version include comparisons of 3D and 2D-axisymmetric simulations [21]. Bubbles rising in a liquid are a good application given the fundamental nature of the phenomenon and the large number of experimental and theoretical studies on the subject [38,39,40]. An interesting problem would be the, as yet unsolved, transition from 2D axisymmetric to 3D helicoidal motion of gas bubbles rising in a liquid [39].

Throughout the project we will keep in mind generality. For example, we will maintain independence between the hydrodynamic and interface discretisations, and the integration procedures for control volumes cut by the interface will be designed generically. We will also favour "good programming" practices in order to obtain not only a specific tool for numerical simulations but also a programming toolbox applicable to a variety of problems (ranging from computational geometry to a variety of interface-related applications).

## 87. REFERENCES

Please list references for Sections 4-6. Use as many pages as necessary. Please include full titles.

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## 9 8. TIMETABLE

9.1

9.2 Number of Years (**maximum of 2**): **2**

Describe in general terms the advances you hope to make in each year. It is acknowledged that this timetable may be revised as the research progresses.

*Year 1:*

Implementation of the interface advection scheme.

Extension and testing of the mesh refinement and coarsening procedures used to control mesh quality.

Implementation of a simplified two-phase flow solver including surface tension but not different physical properties for the two fluids.

Application to simple test cases and validation of the integral and Boolean operations approaches.

*Year 2:*

Generic formulation for the case of contrast in physical properties (density and viscosity).

Implementation starting from the previous simple model.

Validation using the rising bubble test case and comparison with experimental and theoretical predictions.

10

## 11 9. SPECIAL REQUIREMENTS

Describe any special requirements for equipment or resources (e.g., mass spectrometers, laboratories, research ships) and indicate how these will be met. You must demonstrate that you will have the means to complete the research.

N/A

## 12 10. SPECIAL SKILLS

The skills of the Principal and Associate Investigators and other named researchers are included in Section 12. If other staff, particularly postdoctoral researchers, are included in the proposal, indicate here what skills are available or are being sought.

N/A

## 13 11. ETHICAL OR REGULATORY OBLIGATIONS

It is your responsibility to ensure that all ethical or regulatory obligations are met (e.g. from ERMA, MAF, Animal Ethics, Human Ethics). For particular projects, consultation with Maori may be appropriate. Indicate what steps have been, or will be, taken to obtain the necessary approvals. Full documentation needs to be received before any grant is paid.

**14 N/A**

## 12. CURRICULUM VITAE, PUBLICATIONS AND OTHER PUBLISHED WORKS

Use copies of Sections 8a & 8b from your Preliminary Research Proposal renumbering as section 12 and updating if necessary. Please use only one page per person for a CV and preferably one page per person for the list of requested publications. The information needs to be supplied for each named research person (other than research/technical assistants). This includes postdoctoral fellows if a person has already been chosen for the position.

Name of Researcher:	Stéphane Popinet
Tertiary Education:	September 1997-October 2000: PhD in fluid mechanics at the Laboratoire de Modélisation en Mécanique, Université Pierre et Marie Curie, Paris. Supervisor: Stéphane Zaleski. Subject: Numerical simulation of interfaces and free-surfaces and application to cavitation bubble dynamics and sonoluminescence.  1994-1995: DEA (Advanced Studies Diploma) Oceanology, Meteorology and Environment (Option: Geophysical Fluid Dynamics) at the Université Pierre et Marie Curie, Paris.  1993-1994: Final Year at the Ecole Nationale Supérieure d'Arts et Métiers (ENSAM), Paris.  DEA in Mechanics (Option: Fluid Mechanics) at the Université Pierre et Marie Curie, Paris.
Distinctions/Honours:	PhD: mention très honorable avec les félicitations du jury.
Employment Record:	May 2001 - Postdoctoral Fellow, NIWA  August 1995-January 1997: French National Service (''Coopération'') at Schlumberger Cambridge Research (UK) in the Fluid Chemistry and Physics Department. Supervisor: Paul Hammond. Subject: Numerical simulations of liquid-liquid two-phase flows using mixture equations and application to oil extraction.
Other Information:	

14.1.1.1.1

## 15 12B. PUBLICATIONS

|Name of researcher: |Stéphane Popinet

|Indicate total number of books, refereed journal |7 |

|articles or refereed conference papers published | |

List the following: (i) **refereed** publications published since, but not including 1995, and (ii) prior publications that relate directly to the proposal. For each section, please give full titles and separate refereed publications into the following categories: a)journal articles; b)books; c)book chapters; d)books edited; e)refereed conference proceedings.

For each category please list the most recent publications first.

### (i) **Publications (1996 - present)**

#### *Journal articles*

A. Menchaca-Rocha, A. Martinez-Davalos, R. Nunez, S. Popinet and S. Zaleski. Coalescence of liquid drops by surface tension. *Phys. Rev. E*, accepted for publication, 2001.

E. Ory, H. Yuan, S. Prosperetti, S. Popinet and S. Zaleski. Growth and collapse of a vapor bubble in a narrow tube. *Phys. Fluids*, 12:1268-1277, 2000.

S. Popinet and S. Zaleski. A front tracking algorithm for the accurate representation of surface tension. *Int. J. Numer. Meth. Fluids*, 30:775-793, 1999.

P. Carles and S. Popinet. Viscous non-linear theory of Richtmyer-Meshkov instability. *Phys. Fluids*, accepted for publication, 2001.

#### *Refereed conference proceedings*

S. Popinet and S. Zaleski. Bubble collapse near a solid boundary: A numerical study of the influence of viscosity. IUTAM Symposium on Free Surface Flows, Birmingham, UK, July 2000.

S. Popinet and S. Zaleski. Coupling of radial and translational motion in small viscous bubbles. Proceedings of the 4th International Congress on Industrial and Applied Mathematics, Edinburgh, UK, July 1999.

S. Popinet and S. Zaleski. Deformed bubbles in inhomogeneous ultrasonic fields. APS Fluid Mechanics Division Meeting, Philadelphia, USA, November 1998.

S. Popinet and S. Zaleski. Simulation of axisymmetric free-surface viscous flow around a non-spherical bubble in the sonoluminescence regime. Proceedings of the Third International Conference On Multiphase Flow, Lyon, France, June 1998.