



# A second order virtual node algorithm for Navier–Stokes flow problems with interfacial forces and discontinuous material properties



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## ARTICLE INFO

### Article history:

Received 18 June 2013

Received in revised form 20 January 2014

Accepted 27 January 2014

Available online 11 February 2014

### Keywords:

Navier Stokes

Virtual node algorithms

Interface problems

Cartesian grids

## ABSTRACT

We present a numerical method for the solution of the Navier–Stokes equations in three dimensions that handles interfacial discontinuities due to singular forces and discontinuous fluid properties such as viscosity and density. We show that this also allows for the enforcement of normal stress and velocity boundary conditions on irregular domains. The method improves on results in [1] (which solved the Stokes equations in two dimensions) by providing treatment of fluid inertia as well as a new discretization of jump and boundary conditions that accurately resolves null modes in both two and three dimensions. We discretize the equations using an embedded approach on a uniform MAC grid to yield discretely divergence-free velocities that are second order accurate. We maintain our interface using the level set method or, when more appropriate, the particle level set method. We show how to implement Dirichlet (known velocity), Neumann (known normal stress), and slip velocity boundary conditions as special cases of our interface representation. The method leads to a discrete, symmetric KKT system for velocities, pressures, and Lagrange multipliers. We also present a novel simplification to the standard combination of the second order semi-Lagrangian and BDF schemes for discretizing the inertial terms. Numerical results indicate second order spatial accuracy for the velocities ( $L^\infty$  and  $L^2$ ) and first order for the pressure (in  $L^\infty$ , second order in  $L^2$ ). Our temporal discretization is also second order accurate.

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## 1. Introduction

The simulation of multiphase incompressible flow in arbitrary domains is necessary for many applications in computational physics and engineering. Unfortunately, it is particularly difficult to attain orders of accuracy easily achievable in the case of uniform or periodic domains. Due to irregular interface and domain boundary geometries, a natural approach to the numerical approximation of the equations is the finite element method (FEM) with unstructured meshes that conform to the irregular geometry. However, meshing complex interface geometries can prove difficult and time-consuming when the interface frequently changes. We have recently developed a class of embedded methods that utilize uniform Cartesian grids and sub-cell representations of interface/boundary geometry to achieve optimal accuracy without the need for frequent

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remeshing [1–4]. Our use of regular grids simplifies the implementation, permits straightforward numerical linear algebra and naturally allows for higher order accuracy in  $L^\infty$ . We have used the term virtual node methods to describe these techniques since they utilize additional structured degrees that are outside the domain of interest. In the present work, we introduce a new virtual node method for approximating the two-phase Navier–Stokes equations with irregular embedded interfaces and boundaries on a uniform Cartesian Marker and Cell (MAC) grid, where velocity degrees of freedom are located at face centers and pressure degrees of freedom are located at cell centers.

As in [1], we duplicate Cartesian grid cells along the interface  $\Gamma$  to introduce additional virtual nodes that accurately resolve discontinuous quantities. This naturally treats discontinuities in material properties such as viscosity and density. Interface cells are cut and duplicated using a level set that allows for accurate evaluation of integrals needed for the numerical stencils. These stencils (for the viscous stress forces as well as the divergence-free and jump constraints) are constructed from a variational formulation that yields a symmetric linear system. This approach requires the introduction of a Lagrange multiplier variable to maintain continuity of the fluid velocity across the interface. Unfortunately, the introduction of this variable forced the approach in [1] to require that interface domain geometry have a constant normal on each MAC grid cell. Although it is a reasonable restriction in two dimensions, this is not possible in three dimensions and so the method was fundamentally limited to 2D. We present an improved discretization of this Lagrange multiplier term that works naturally in both two and three dimensions without the restriction of a constant normal per MAC grid cell. The necessity of this in [1] was due to the requirement that the discretization resolve null modes in the variational form of the equations exactly. Failure to do this resulted in significant degradation in performance. We show that our new discretization also captures these modes exactly.

We also consider a simplification to the combination of the second order Backward Difference Formula (BDF) and second order semi-Lagrangian schemes that are often used in second order Navier–Stokes discretizations to calculate the intermediate velocity field [5]. This simplification reduces the number of semi-Lagrangian interpolation steps required from four to two while retaining the temporal and spatial accuracy of the original method. The interface is evolved using the level set method or, when more appropriate, the particle level set method. Numerical experiments indicate second order accuracy in  $L^\infty$  and  $L^2$  for the velocity and first order accuracy in  $L^\infty$ , second in  $L^2$ , for pressure. Numerical experiments indicate a stability restriction on the *minimum* time step size (relative to the grid spacing) that may be taken by our method in the case of a Navier–Stokes discretization. We explore the nature and source of this restriction further.

## 2. Existing methods

In our discussion of existing approaches, we will focus only on embedded (or immersed) methods that avoid unstructured meshing when addressing boundary and interface conditions at irregular geometric boundaries. Embedded methods place an irregular domain, or a domain with an interface, into a rectangular computational domain with a Cartesian grid. A good review of such methods is given by Lew et al. in [6]. A classic embedded method is the Immersed Boundary Method (IBM) developed by Peskin [7–12] originally to simulate blood flow in the heart. The IBM uses regularized delta functions to represent singular forces acting on interfaces. This renders the method first order accurate in general for thin interfaces, implying that the physical characteristics of the flow near those interfacial boundaries are not accurately captured [13]. For interfaces with a nonzero thickness, modifications to the IBM can yield second-order accuracy [14]. The original IBM also featured poor volume conservation near the interface, motivating the development of a volume-conserving version in [15]. However, the IBM has proven very useful for many applications.

Many methods have been developed to improve on the performance of the IBM. Mittal and collaborators have shown that a discrete forcing (rather than one first applied to the continuous equations and then discretized) can be used to get second order accuracy for flows in irregular domains [16–19]. The Immersed Interface Method (IIM) [13,20–23] is a popular example that attains second order accuracy in  $L^\infty$  by modifying the numerical stencil near the interface, and by using jump conditions instead of regularized delta functions to relate the singular forces to interfacial discontinuities in pressure, velocities and their derivatives. The IIM has been used in simulating interfaces between fluids with different viscosities [24–27] and has been extended to higher-order implementations [28,29]. The IIM is considerably more difficult to implement than the IBM and most applications are in two space dimensions as a result. However, researchers have applied the IIM to three-dimensional flows [30]. Recent IIM approaches use adaptive grid techniques near the interface to maintain high resolution near the important parts of the boundary while reducing the overall degrees of freedom [31]. In general, the IIM yields non-symmetric linear systems, and therefore requires the use of solvers such as GMRES or BiCG-STAB. Some implementations of IIM [32] yield symmetric positive definite systems, however this is only possible when the viscosity is continuous across the interface. The Matched Interface and Boundary (MIB) method [29,33] adjusts the approach of the IIM with dimension-by-dimension modifications that utilize fictitious points. Enforcement of jump conditions is decoupled from the modified finite difference stencil. The work of [34] applies the framework of the MIB to interfacial flow in two dimensions.

Our approach was initially motivated by The Ghost Fluid Method (GFM). However, because that method does not in the end introduce any additional degrees of freedom into the discretization, we used the term from another of Fedkiw's methods [35] that does similarly introduce virtual degrees of freedom. Notably, the GFM always guarantees a symmetric discretization. Initially applied to the Poisson equation with interfacial jumps and variable coefficients [36], the GFM was also used to simulate multiphase incompressible flow in [37]. Unfortunately, the GFM is only capable of achieving first order

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