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# Hybrid grid–particle methods and Penalization: A Sherman–Morrison–Woodbury approach to compute 3D viscous flows using FFT

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ABSTRACT

Particle methods are very convenient to compute transport equations in fluid mechanics as their computational cost is linear and they are not limited by convection stability conditions. To achieve large 3D computations the method must be coupled to efficient algorithms for velocity computations, including a good treatment of non-homogeneities and complex moving geometries. The Penalization method enables to consider moving bodies interaction by adding a term in the conservation of momentum equation. This work introduces a new computational algorithm to solve implicitly in the same step the Penalization term and the Laplace operators, since explicit computations are limited by stability issues, especially at low Reynolds number. This computational algorithm is based on the Sherman–Morrison–Woodbury formula coupled to a GMRES iterative method to reduce the computations to a sequence of Poisson problems: this allows to formulate a penalized Poisson equation as a large perturbation of a standard Poisson, by means of algebraic relations. A direct consequence is the possibility to use fast solvers based on Fast Fourier Transforms for this problem with good efficiency from both the computational and the memory consumption point of views, since these solvers are recursive and they do not perform any matrix assembling. The resulting fluid mechanics computations are very fast and they consume a small amount of memory, compared to a reference solver or a linear system resolution. The present applications focus mainly on a coupling between transport equation and 3D Stokes equations, for studying biological organisms motion in a highly viscous flows with variable viscosity.



## 1. Introduction

Particle methods have been widely studied in the last decades to compute transport equations in fluid mechanics. In their Lagrangian form the associated convective terms are vanishing with the corresponding CFL stability condition [15,4,2], so large time steps can be performed. Moreover Lagrangian methods are linearly scaling, robust and accurate [18,31]. These features are particularly interesting for large 3D computations. Nevertheless, efficient numerical methods are required to compute the related velocity field, in order to keep the Lagrangian treatment of the convection beneficial.

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Indeed, on the one hand, when considering vortex methods based on vorticity, Poisson equations are involved in the velocity computation. Such Poisson equations can be solved using FFT-based or finite differences based solvers [14], or kernel methods improved by multipole development techniques [12]. FFT-based solvers provide excellent efficiency even for very large flows [6], particularly for unbounded or periodic domains with no obstacles [7]. Kernel methods (such as Biot–Savard laws for the Poisson equation or Stokeslets for the Stokes equation) are usually less efficient, but they can handle boundaries naturally using integral equations on surfaces [32], and are well fitted for infinite domain problems [30]. Their main drawback is that the expression of the kernel for variable flow parameters (such as viscosity) does not exist, and therefore these methods cannot be applied.

On the other hand, whether a Poisson equation or another elliptic model is involved for the velocity computation, standard discretization methods, such as finite elements or finite volumes methods [17], are leading to large non-standard linear systems [38], whose assembling and resolution become prohibitive for large 3D flows. Furthermore, these problems become especially challenging when the fluid is interacting with immersed moving objects and when the fluid inner composition is not homogeneous.

The Penalization method introduced by Angot et al. [3] is an interesting way to handle the fluid–structure interaction by adding a term in the conservation of momentum equation. Moving obstacles are considered through their characteristic function so a single mesh is used and no remeshing is needed. A splitting of Navier–Stokes equations enables to compute separately the convection (with Lagrangian methods), the diffusion and the Penalization. For high Reynolds numbers diffusion does not dominate so the associated stability condition does not restrict the method: computations can be explicit [23,13]. When the Reynolds number becomes smaller, this CFL condition imposes smaller time steps and implicit computations are required to keep using Lagrangian methods efficiency (with large time steps). It becomes critical when the Reynolds number is so small that the flow is governed by quasi-static Stokes equations: both the Penalization and the diffusion have to be computed together.

This article presents a novel approach to compute implicitly this Penalization term, which is crucial for the stability and the convergence of algorithms. The present method is based on the Sherman–Morrison–Woodbury (SMW) formula (1), which allows to compute the inverse of a perturbed matrix $A + E^T C E$ with respect to the original inverse matrix $A^{-1}$, by means of the following relation:

$$\left(A + E^T C E\right)^{-1} = A^{-1} - A^{-1} E^T \left(C^{-1} + E A^{-1} E^T\right)^{-1} E A^{-1} \qquad (1)$$

One can refer for instance to [25] for a review of history, various uses and extensions of this formula.

In this equation $A$ and $C$ are square matrices of size $n$ and $p$ respectively while $E$ is a $p$ by $n$ matrix. $p$ is the rank of the perturbation and is assumed to be smaller than $n$. This is an algebraic relation, which leads to two features: on the one hand no approximation is made to get this formula (and consequently no error is added); on the other hand this allows coefficients of $C$ to be as large as needed, hence the method fits very well for Penalization coefficients which jump from zero to $1/\varepsilon$.

This new method aims at being cheap from a computational point of view so matrix assembling and linear system resolution are avoided. The Penalization term is treated as a small rank perturbation and the SMW formula is exploited coupled to a GMRES approach to get a numerical algorithm which involves only Poisson problems resolution. In this way fast solvers based on Fast Fourier Transforms are used and the computational cost stays reasonable even for large 3D problems. It is shown that the computational cost of the problem computed with this new numerical method is not depending on the complexity of the geometry. This is a good alternative to Kernel methods such as Stokeslets (whose computational time is directly linked to the number and size of obstacles) and linear system assembling (since the condition number grows dramatically with the number of penalized points). This paper shows that this novel method enhanced computational performances: less memory is consumed and computations are faster than using direct multigrid solvers or linear system resolutions.

In Section 2, the Penalization method is presented for the Poisson equation. We present our novel methodology and the computational benefits on this simple problem before introducing the method in the context of fluid mechanics equations. In Section 3, the numerical algorithm to solve the Stokes problem with variable viscosity in a complex geometry is presented coupled to a Lagrangian method for transport equations. The chosen splitting makes appear exactly penalized Poisson problem so the methodology developed in Section 2 is straightly applied. In Section 4, three numerical fluid mechanics illustrations, including applications to biomedical computing, are presented. Finally in Section 5 the computational performances are discussed for these different fluid mechanics simulations.

## 2. Penalized problems and use of Sherman–Morrison–Woodbury (SMW) formula

### 2.1. Problem setup for penalized Poisson equation

The method is first presented for a Poisson problem and generalized in the following for fluid mechanics equations. Let $u$ be the solution to a penalized Poisson equation in a domain $\Omega$, with homogeneous Dirichlet boundary conditions imposed on $\partial\Omega$: