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A Neumann–Neumann preconditioned iterative substructuring approach for computing solutions to Poisson's equation with prescribed jumps on an embedded boundary

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ABSTRACT

In multifluid problems with surface tension the fluid pressure and its derivative are discontinuous at fluid interfaces. We present a Cartesian grid embedded boundary method for numerically resolving these discontinuities in which we use Neumann–Neumann preconditioned iterative substructuring to solve the governing equations. We validate this method by computing several well-known Poisson problems with discontinuous coefficients, and we compare its performance to an approach based on simple iteration. By analogy with the conjugate gradient method, we hypothesize that the scaling of the Neumann–Neumann preconditioned iterative substructuring is $O(h^{-D} \ln h^{-1})$ where *h* is the cell size and D = 2, 3 is the dimensionality of the problem. In contrast, we show that the simple iterative procedure scales like $O(h^{-(D+1)})$ and is slower by a factor of 4000 for a small (i.e., 64×64 cell) model calculation with physical parameters corresponding to a 1.5 mm air bubble in water. We present an analytical model to explain the scaling of this iterative procedure.

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1. Introduction

This work is motivated by the goal of modeling the interface between two fluids in incompressible two-phase flow on uniform Cartesian grids in which the fluid interface is represented as an embedded boundary in those cells that intersect the interface. The equations governing incompressible two-phase flow are subject to jump conditions at the fluid interface in which both the pressure and its gradient are discontinuous while the velocity is continuous but has a discontinuous gradient. Consequently, differential operators in the momentum equations, such as the gradient and the Laplacian, become unbounded in regions abutting the interface. This problem is often addressed by regularizing or 'smoothing' the operator or its discretization. However such smoothing introduces an additional computational parameter that governs the size of the region over which the operator is regularized, which, if the computed solution is to converge to the true solution of the problem, must also go to zero as the grid size goes to zero. This approach also leads to a region in a neighborhood of the interface over which values of quantities defined on the interface are spread out or 'smeared' resulting in a representation of the interface that is not sharp.

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Here we study an alternate approach in which we discretize each of the fluid domains Ω_1 , Ω_2 separately so the governing equations are well-defined within each domain and the discontinuities or jumps in the dependent variables become boundary conditions on the boundary, $\partial\Omega_{12} = \partial\Omega_1 \cap \partial\Omega_2$, between the two domains. This approach is attractive for several reasons. It builds on well-established single domain computational algorithms for solving the governing partial differential equations (PDEs) in a single fluid domain. It also provides a sharp representation of the interface, thereby allowing better resolution of gradients normal to the interface leading to, for example, improved accuracy of algorithms for modeling the transport of quantities across interfaces, as well as more accurate models of quantities such as surfactants, that flow on the interface itself.

In this article we examine two approaches for coupling implicit Poisson solvers with jump boundary conditions in the context of a finite volume discretization of the governing PDEs on Cartesian grids, in which we use the embedded boundary approach to model irregular geometries such as a fluid interface. One of these approaches is the algorithm of Crockett et al. [6] (CCG), which synchronizes boundary conditions between the two domains with each *V*-cycle of a multigrid solver. In our approach, which is based on the so-called iterative substructuring method, we use an iterative Krylov space method to directly determine the boundary conditions on the interface $\partial \Omega_{12}$ between the two domains. We will refer to this latter approach as NNIS, for *Neumann–Neumann preconditioned iterative substructuring*. Both approaches use the same discretization of the governing PDE, the same boundary condition stencils, and identical multigrid solvers.

1.1. The governing equations

Incompressible two-phase flow is governed by the following momentum and continuity equations,

$$\frac{\partial}{\partial t} \mathbf{v}_{\alpha} + \mathbf{v}_{\alpha} \cdot \nabla \mathbf{v}_{\alpha} + \frac{1}{\rho_{\alpha}} \nabla P = v_{\alpha} \Delta \mathbf{v}_{\alpha} + \frac{1}{\rho_{\alpha}} \nabla \cdot \boldsymbol{\tau}_{\alpha},$$
(1a)
$$\nabla \cdot \mathbf{v}_{\alpha} = \mathbf{0},$$
(1b)

where we have used the subscript $\alpha = 1,2$ to distinguish between phase or fluid 1 and 2. In (1) **v** is the velocity, *P* the pressure, ρ the density, *v* the kinematic Newtonian viscosity, and τ is an extra stress that one can use describe, for example, non-Newtonian rheology such as viscoelasticity.

The surface tension between the two phases results in a force per unit area, **f**, on the surface of the interface $\partial \Omega_{12}$, which is given by

$$\mathbf{f} = -\sigma \kappa \mathbf{n}_1,\tag{2}$$

where σ is a phenomenological coefficient, κ is the curvature of the interface, and **n** is a unit vector normal to $\partial\Omega_{12}$. We employ the convention that **n**_{α} is the outward-directed unit normal on $\partial\Omega_{\alpha}$ and hence, **n**₂ = -**n**₁ on $\partial\Omega_{12}$.

Let ψ be a level set function such that the zero contour $\psi = 0$ coincides with the interface. Then the curvature κ of the interface is given by

$$\kappa = \nabla \cdot \left(\frac{\nabla \psi}{|\nabla \psi|} \right). \tag{3}$$

We choose the sign convention $\psi < 0$ in Ω_1 , which fixes a sign convention for σ .

For the problem (1), (2) with σ constant (i.e., no Marangoni forces), the boundary conditions on the pressure *P* are given by,

$$\llbracket P \rrbracket = \llbracket \tau_{nn} \rrbracket + \mathbf{n}_1 \cdot \mathbf{f}. \tag{4a}$$

$$\left[\!\left[\frac{1}{\rho}(\mathbf{n}_{1}\cdot\nabla)P\right]\!\right] = \left[\!\left[\frac{1}{\rho}\mathbf{n}_{1}\cdot(\nabla\cdot\boldsymbol{\tau})\right]\!\right] + \left[\!\left[\mathbf{n}_{1}\cdot\nu\Delta\mathbf{v}\right]\!\right],\tag{4b}$$

where the notation $[\![\phi]\!]$ denotes the jump $\phi_2 - \phi_1$ on $\partial\Omega_{12}$. The boundary conditions on the velocity are

$$\begin{bmatrix} \mathbf{v} \end{bmatrix} = \mathbf{0},$$

$$\begin{bmatrix} (\mathbf{n}_1 \cdot \nabla) (\mathbf{v} \cdot \mathbf{n}) \end{bmatrix} = \mathbf{0},$$

$$(5b)$$

$$\llbracket \rho v(\mathbf{n}_1 \cdot \nabla) \mathbf{v} \rrbracket = -\mathbf{n}_1 \cdot \llbracket \tau \rrbracket + \llbracket \tau_{nn} \rrbracket \mathbf{n}_1.$$
(5c)

A Hodge decomposition (e.g., see [5]) of the momentum Eq. (1a) yields the governing equation for the pressure in each phase:

$$\Delta P = \nabla \cdot (\nabla \cdot \boldsymbol{\tau} + \rho[v \Delta \mathbf{v} - \mathbf{v}_t - \mathbf{v} \cdot \nabla \mathbf{v}]). \tag{6}$$

We solve (6) on Ω_1 and Ω_2 separately, with the boundary conditions (4a,b) coupling the two single-phase solutions (e.g., see Fig. 1). Although the domains are time dependent, discretizations of the time-dependent problem can be based on fixed-time solutions of (6) (e.g., see [23]). Similarly, with operator splitting the viscous operator in (1a) can be discretized using a sequence of Helmholtz operators at discrete time intervals with jump conditions (5) (see [23]).

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