A low-cost space-time finite element for free-surface flows under total Lagrangian description

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Abstract. In this work, we propose a position-based space-time finite element formulation for incompressible Newtonian flows under a total Lagrangian description. This formulation is suggested within the context of finite strain free-surface flows and differs from the traditional finite element approach for fluid dynamics by utilizing current nodal positions as the main variables instead of nodal velocities. In contrast to time-marching methods, space-time formulations involve applying the finite element technique not only to the spatial domain but also to the temporal domain. The proposed approach employs a finite element discretization that can be unstructured or structured in space, but is always structured in time. Thus, the space-time shape functions are expressed as a tensor product of linear shape functions in the spatial direction and specially designed quadratic shape functions in the temporal direction. Consequently, the space-time domain is divided into time slabs that are solved progressively, with the final velocities and positions from the previous time slab serving as initial conditions for the current one, thereby reducing the dimension of the discrete system of equations. The proposed shape functions in the temporal direction yield a system of equations of the same size as standard time-marching methods, but with advantages stemming from the space-time discretization: different stability and high-frequency dissipation can be achieved based on the selection of the time test functions. To solve the incompressible problem stably, we employ mixed equal-order position-pressure finite elements with Petrov-Galerkin/pressure stabilization (PSPG). This formulation possesses several significant features that justify its development: 1) the space-time formulation facilitates dynamic re-meshing by permitting the spatial discretization at the end of one time slab to differ entirely from the spatial discretization at its beginning, thus extending its applicability to flows with undefined distortion and topological changes; 2) by considering positions as variational parameters, it becomes straightforward to couple with Lagrangian hyper-elastic solid solvers, which may also be formulated in terms of positions or displacements in a monolithic way. Numerical example conducted to validate the formulation demonstrate its robustness and efficiency for finite strain free surface flows, including phenomena such as sloshing.

Keywords: Space-Time methods, Total Lagrangian description, Free-Surface Flows.

1 Introduction

The Finite Element Method has been successfully used in the context of incompressible fluid dynamics under the Eulerian description, where the unknowns are the nodal velocities and pressures, as one can see from Hughes et al. [1], Tezduyar et al. [2], and Tezduyar et al. [3]. However, the Eulerian formulation has some limitations, such as the need for stabilization techniques to prevent spurious oscillations arising from the convective terms present in the governing equations, as well as its inability to be directly applied to moving boundary flows, as it is developed over a fixed domain. A robust approach for moving-boundary flows is the Arbitrary Lagrangian-Eulerian (ALE) formulation [4], which allows for dynamic mesh movement independent of the fluid motion. However ALE solvers cannot be directly applied to problems with very large distortions in the fluid domain or with topological changes in the domain, unless they are combined with re-meshing techniques.

Another option for free-surface flows is to employ the Lagrangian description, which avoids the convective terms from the Navier-Stokes equations at the same time that automatically solves the free-surface position problem. This approach also simplifies the monolithic coupling with structures and enhances efficiency in fluid-structure interaction problems Idelsohn et al. [5]. This kind of method can be directly applied free surface flows with finite distortions, however, the combination with re-meshing is necessary for large distortions, that may lead to mesh entanglement and specially to cases with topological changes of the fluid domain.

Some authors have developed methods using the updated Lagrangian description, such as Radovitzky and Ortiz [6] and Onate and Carbonell [7], using velocity as the main variable, updating coordinates through an additional numerical integration procedure over time. Avancini and Sanches [8] introduces a total Lagrangian position-based formulation for incompressible flows. The position-based approach is more compact than displacement-based formulations and eliminates the need for the position update step required in velocity-based formulations. However, the total Lagrangian framework is limited to cases of flows with finite deformations, as the update of the reference in necessary when re-meshing is applied.

In dynamic scenarios, time-marching methods are frequently employed to solve systems of ordinary differential equations resulting from any spatial discretization technique. A widely recognized implicit time-stepping approach is the average acceleration method, which is a variant of Newmark's method Newmark [9]. In contrast to time-stepping methods, Space-Time (ST) formulations, developed initially by Hughes and Hulbert [10], apply the finite element method across both spatial and temporal domains. This approach is known for its advantages in stability and accuracy, especially in modeling problems within fixed spatial domains. Over time, the methodology has been refined and effectively used in a wide array of time-dependent issues. These include linear and nonlinear elastodynamics Dumont et al. [11], structural problems involving continuous damage mechanics Wada et al. [12], fluid-structure interactions Bazilevs et al. [13], and fluid flow scenarios von Danwitz et al. [14].

Structured space-time meshes extend a spatial discretization into the temporal dimension, resulting in a discretization with space-time prismatic elements formed by the Cartesian product of spatial and temporal finite elements. This approach resembles time-marching methods, allowing solutions to be sequenced and information to propagate along the positive time axis. In contrast, using unstructured meshes allows the problem to be solved in one step without the need for sequencing, which can be advantageous for problems with complex geometries and topological changes, but is significantly more computationally expensive due to the high-dimensional mesh. According to Foteinos and Chrisochoides [15], a 4D mesh (3D spatially) is approximately 100 times slower than a 3D mesh when using Delaunay triangulation.

In this work we present a position-based space-time finite element formulation for incompressible Newtonian free-surface flows under a total Lagrangian description. This formulation is introduced in the context of finite distortion free-surface flows and should be modified in future works to be extended to more complex problems.

The proposed approach employs a finite element discretization that can be unstructured or structured in space, but is always structured in time, with specially designed quadratic shape functions in the time direction, enabling progressive solution and resulting a method with similar computational costs to the standard time-marching approaches.

1.1 Governing Equations in the Total Lagrangian Description

The governing equations for newtonian incompressible flows in the total Lagrangian description can be found in Avancini and Sanches [8], and are given by the boundary and initial values problem defined over the space-time domain $Q = \Omega \times (0, T)$:

$$\nabla \cdot \mathbf{P}^T + \mathbf{b}_n = \rho \ddot{\mathbf{y}} \quad \text{in } \Omega \times (0, T), \tag{1}$$

$$J - 1 = 0 \quad \text{in } \Omega \times (0, T), \tag{2}$$

$$\mathbf{y}(\mathbf{x}, 0) = \overline{\mathbf{y}}(\mathbf{x}, 0) \quad \text{in } \Gamma^D \times (0, T), \tag{3}$$

$$\mathbf{P} \cdot \mathbf{n}_0 = \mathbf{t}_0 \quad \text{on } \Gamma^N \times (0, T) \tag{4}$$

and

$$\mathbf{y}(\mathbf{x}, 0) = \mathbf{y}_0(\mathbf{x}) \quad \text{on } \Omega, \tag{5}$$

where $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor, $\mathbf{y}$ represents the current coordinates, $\mathbf{b}_n$ the volumetric force per unit reference volume, ρ the mass density, $\ddot{\mathbf{y}}$ the material point acceleration field, J the Jacobian determinant of the deformation function, $\mathbf{n}_0$ the normal unity vector to the boundary in the initial configuration, $\mathbf{t}_0$ the traction vector on the Neumann boundary regarding the initial configuration, and $\mathbf{y}_0$=$\mathbf{x}$ the initial coordinates. Ω represents the initial spatial domain, T the final instant, Γ^N and Γ^D the initial Neumann and Dirichlet boundary, respectively.

The constitutive law for incompressible Newtonian flows, in the Lagrangian reference framework, is given by (see Avancini and Sanches [8]):

$$\mathbf{S} = \mathbf{S}' - pJ\mathbf{C}^{-1} = \mathcal{D}_0 : \dot{\mathbf{E}} - pJ\mathbf{C}^{-1} \tag{6}$$

where $\mathbf{S}$ is the second Piola stress tensor, $\mathbf{S}'$ is the deviatoric part of $\mathbf{S}$, p is the pressure, $\mathcal{D}_0$ is the constitutive tensor in the Lagrangian reference, $\dot{\mathbf{E}}$ is the rate of the Green-Lagrange strain tensor and $\mathbf{C}$ is the right Cauchy Green stretch.

The Green-Lagrange strain is an objective Lagrangian measure of strain given by:

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I}) = \frac{1}{2}(\mathbf{C} - \mathbf{I}), \tag{7}$$

where $\mathbf{F} = \nabla_{\mathbf{x}}\mathbf{y}$ is the deformation gradient. Therefore, the rate of Green-Lagrange strain is given by:

$$\dot{\mathbf{E}} = \frac{D}{Dt}(\mathbf{E}) = \frac{1}{2}(\dot{\mathbf{F}}^T\mathbf{F} + \mathbf{F}^T\dot{\mathbf{F}}). \tag{8}$$

The second Piola stress tensor $\mathbf{S}$ is related to the first Piola stress tensor $\mathbf{P}$ and to the cauchy stress tensor $\boldsymbol{\sigma}$ by:

$$\mathbf{S} = \mathbf{F}^{-1}\mathbf{P} = J\mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-T}. \tag{9}$$

2 Space-Time Finite Element Formulation

Unlike standard finite element with time-marching methods, where integrations are performed over the spatial domain and then the corresponding temporal approximations were made, in the space-time finite element context the space an time dimensions are both discretized by finite elements, with space-time shape functions.

In the case of space-time finite element methods with structured time discretization, the discrete problem can be subdivided into a number of space-time slices Q_n, which are constructed between time levels n and $n+1$. Consequently, the space-time domain divided into time slabs can be solved progressively, with the final velocities and positions from the previous space-time slice serving as initial conditions for the current one, and thereby reducing the dimension of the discrete system of equations. As our formulation is described in terms of the initial spatial configuration, we need to define an support space-time slab Q_n^0 for purpose of integration, which is defined by the slice of a regular extrusion of the initial configuration Ω_0 along time direction.

For time-structured space-time meshes, the vector of space-time shape functions $\mathbf{N}$ can be constructed by the tensor product of spatial shape functions vector $\boldsymbol{\phi}$ with temporal shape functions $\boldsymbol{\psi}$, so that, in an index notation we can write:

$$N_a^\alpha = \phi_a(\boldsymbol{\xi}) \otimes \psi^\alpha(\theta), \tag{10}$$

where ϕ_a are the shape functions associated to each spatial node a, and $\psi^\alpha$the shape functions associated to each temporal node α, $\boldsymbol{\xi}$ is the vector of non-dimensional support coordinates in space direction and θ is the non-dimensional coordinate in time direction. In this way, a space-time node can be defined by the indexes pair (a,α), and the spatial and temporal discretizations can be decoupled.

In this work, we restrain our attention to 2D spatial cases, so that the space-time finite element is constructed by the product of a triangular element for spatial discretization with a line element for temporal discretization, resulting into a prismatic space-time finite element with triangular basis and height in the time direction.

For spatial discretization, we use linear shape functions for approximating position and pressure, however, in time direction we need to be able to represent the second derivative os position (acceleration), so that we design special quadratic shape functions for interpolating position trial solution, while we keep constant time approximation for representing the pressure trial solution.

Thus, the functions that represent the initial configuration of the fluid is given by $\mathbf{x}^h(\boldsymbol{\xi}) = \phi_a(\boldsymbol{\xi})\mathbf{x}_a$, where $\mathbf{x}_a$ is the initial coordinate of spatial node a, while the current configuration of any arbitrary point within the time-slice Q_n is given by:

$$\mathbf{y}^h(\boldsymbol{\xi},\theta) = \underbrace{\phi_a(\boldsymbol{\xi})\ \psi^\alpha(\theta)}_{N_a^\alpha(\boldsymbol{\xi},\theta)}\ \boldsymbol{\Upsilon}_a^\alpha = \phi_a(\boldsymbol{\xi})\ \mathbf{y}_a^t(\theta) \tag{11}$$

where $\boldsymbol{\Upsilon}_a = \{\mathbf{y}_a^n, \mathbf{y}_a^{n+1}, \dot{\mathbf{y}}_a^n\}$ corresponds to the vector of nodal parameters of spatial node a in the time slice Q_n and $\dot{\mathbf{y}}_a^n$ is the velocity of the spatial node a at instant n (i.e., velocity of space-time node (a, n). We can write the position of spatial node a along time, $\mathbf{y}_a^t(\theta)$, as:

$$\mathbf{y}_a^t(\theta) = \psi_1(\theta)\mathbf{y}_a^n + \psi_2(\theta)\mathbf{y}_a^{n+1} + \psi_3(\theta)\dot{\mathbf{y}}_a^n \tag{12}$$

The pressure trial function within a space-time slice Q_n is given by:

$$p^h(\boldsymbol{\xi},\theta) = \phi_a(\boldsymbol{\xi})p_a^{n+1}. \tag{13}$$

Although other possibilities for pressure can be explored, in this work we make this choice seeking the smallest computational cost.

2.1 Space-time finite element formulation for incompressible flows

Applying the weighted residual method to Eqs. (1) and (2), integrating over the space-time domain Q_n^0, we formulate the problem as follows: find the pair of trial functions $(\mathbf{y}^h, p^h) \in \mathcal{S}_\mathbf{y}^h \times \mathcal{S}_p^h$ such that for all test functions $\mathbf{w}^h \in \mathcal{V}_\mathbf{y}^h$ and for all test functions $\mathbf{q}^h \in \mathcal{V}_p^h$, the following relations are satisfied:

$$\int_{(Q_n^0)^h} (\boldsymbol{\nabla}_\mathbf{x} \cdot (\mathbf{F}^h\mathbf{S}^h) + \mathbf{b_0} - \rho\ddot{\mathbf{y}}^h) \cdot \mathbf{w}^h d(Q_n^0)^h \tag{14}$$

$$= \int_{t_n}^{t_{n+1}} \int_{\Omega_0^h} (\boldsymbol{\nabla}_\mathbf{x} \cdot (\mathbf{F}^h\mathbf{S}^h) + \mathbf{b_0} - \rho\ddot{\mathbf{y}}^h) \cdot \mathbf{w}^h d\Omega_0^h dt = 0$$

and

$$\int_{(Q_n^0)^h} (J^h - 1)q^h\ \ d(Q_n^0)^h = \int_{t_n}^{t_{n+1}} \int_{\Omega_0^h} (J^h - 1)q^h\ \ d\Omega_0^h dt = 0 \tag{15}$$

The finite-dimensional trial spaces $\mathcal{S}_\mathbf{y}^h$ and $\mathcal{S}_p^h$ and test spaces $\mathcal{V}_\mathbf{y}^h$ and $\mathcal{V}_p^h = \mathcal{S}_p^h$ comprise suitably differentiable functions to effectively approximate the mentioned functions. It is worth mentioning that, due to the sequential and structured temporal integration, it is possible to perform spatial and temporal integrations independently.

The trial functions for momentum and incompressibility equations (Eqs. (14) and (15)) within one space-time slice Q_n^0 are given by:

$$\mathbf{w}^h(\boldsymbol{\xi},\theta) = \phi_a(\boldsymbol{\xi})\ \psi^\alpha(\theta)\mathbf{w}_a^\alpha \tag{16}$$

and

$$q^h(\boldsymbol{\xi},\theta) = \phi_a(\boldsymbol{\xi})q_a^{n+1} \tag{17}$$

2.2 Ladyzhenskaya-Babuška-Brezzi Conditions

For incompressible flows, using the same shape function for the spatial interpolation of positions and pressure does not satisfy the Ladyzhenskaya-Babuška-Brezzi (LBB) conditions [16]. To enable the application of the same approximation for both fields, the Pressure Stabilized Petrov-Galerkin (PSPG) method is employed by adapting the method initially developed for Eulerian formulations [17] to the Lagrangian formulation presented in [8]. To keep the equations concise, we will omit the stabilization terms from the equations, however they are important to ensure consistent pressure fields.

2.3 Slice by Slice Solution Procedure

Lets consider only the first space-time slice Q_0. Notice that the initial conditions $\mathbf{y}_0$ and $\dot{\mathbf{y}}_0$ need to be satisfied, meaning that the first and the last unknowns of nodal position in Eq. (12) are known. In this way, we can solve sequentially each space-time slice, applying the position and velocity field calculated at the end of the previous space-time slab as initial conditions to the current one.

To enforce the initial conditions and get a defined system when solving the problem for Q_n^0, we set the test functions parameters $\mathbf{w}_a^n$ and $\mathbf{w}_a^{n+1}$ in Eq. (16) to zero, similarly to the strategy developed by Mergel et al. [18] in the solid mechanics context, so that, giving the arbitrariness of $\mathbf{w}_a^{n+1}$, Eq. (14) becomes

$$\int_{t_n}^{t_{n+1}} \left(\int_{\Omega_0^h} \rho \phi_a \ddot{\mathbf{y}}^h + (\mathcal{D}_0^h : \dot{\mathbf{E}}^h) \cdot (\mathbf{F}^h)^T : \frac{\partial \phi_a}{\partial \mathbf{x}} - p^h J^h (C^h)^{-1} \cdot (\mathbf{F}^h)^T \right. \\ \left. - \int_{\Gamma_0^h} \mathbf{t}_0^h \phi_a d\Gamma_0^h - \int_{\Omega_0^h} \mathbf{b}_0^h \phi_a d\Omega_0^h \right) \cdot \psi_3 \; dt = 0. \tag{18}$$

Considering the arbitrariness of q_a^{n+1}, eq. (15) becomes:

$$\int_{t_n}^{t_{n+1}} \int_{\Omega_0^h} (J^h - 1)\phi_a \;\; d\Omega_0^h \, dt = 0. \tag{19}$$

Notice that this procedure results a nonlinear system with the same number of degrees of freedom as the one obtained with standard time-marching methods. The integration is performed numerically using Hammer quadrature points in the spatial direction and Gauss quadrature points in the time direction, and the nonlinear system of equations is solved iteratively with Newton-Raphson method.

3 Numerical example - Slosh with small amplitude

This example consists on the simulation of a small amplitude sloshing problem, avoiding the need for remeshing. The initial geometry and data are presented in Fig. 1.

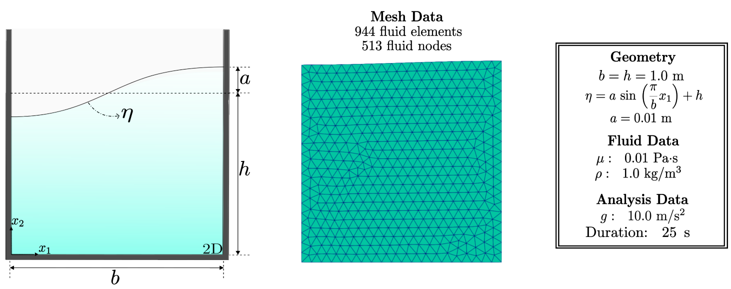


Figure 1. Initial geometry and problem data

To verify the proposed formulation, we consider different time steps (height of the space-time slice): $\Delta t = 0.002$, 0.008, 0.032, and 0.128), while keeping the spatial discretization with 944 elements and 513 nodes. The vertical position of the free surface at the right wall along time is in Fig. 2, where it is compared to the results

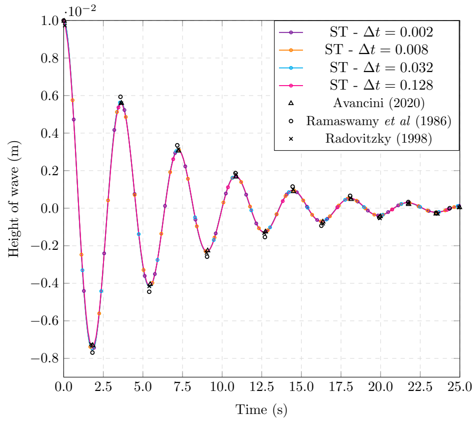
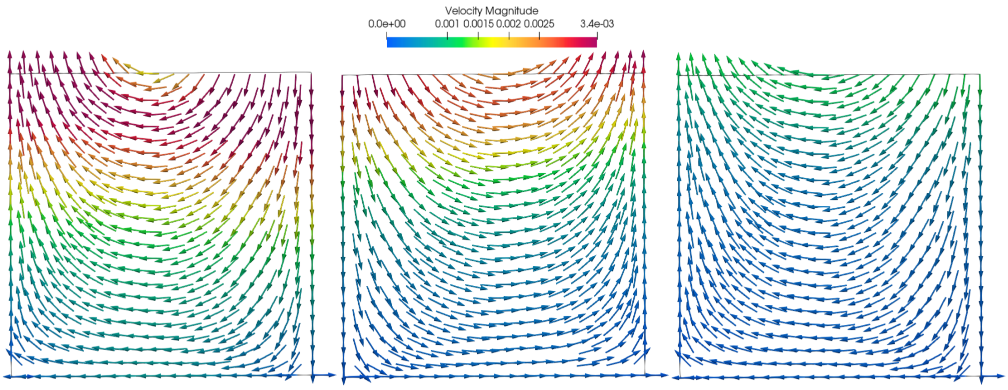


Figure 2. Wave height on the right wall - Analysis considering four different time steps and comparison with literature results.

from [19], [6], and [20] that employed time marching methods, showing good agreement. Snapshots of velocity for different instants are shown in Fig. 3.



(a) 5 s (b) 10 s (c) 15 s

Figure 3. Snapshots of velocity distribution for different instants.

4 Conclusions

This study has introduced a total Lagrangian space-time finite element formulation for simulating free-surface flows under finite strains. The formulation stands out by utilizing current nodal positions and pressure as primary variables, diverging from traditional velocity-pressure-based finite element methods in fluid dynamics. The solution of the space-time problem is performed progressively and the order of the nonlinear system to be solved for each time advance step is the same as the one for standard time-marching methods, leading to similar computational cost.

By utilizing positions as variational parameters, the monolithic coupling with Lagrangian hyper-elastic solid solvers becomes direct, thereby broadening the formulation's applicability to a wider range of fluid-structure interaction problems.

As shown in the numerical example, this formulation has been verified against literature confirmed the expected efficiency. In future studies this method shall be extended to updated Lagrangian description and associated to re-meshing procedures to enable applications at any distortion scale, including problems with topological changes, and also coupled to solid dynamic solver.

Acknowledgements. This study was financed in part by the Sao Paulo Research Foundation (FAPESP) - Process

Number 2021/07516-9, by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - finance code 001 and by Brazilian National Council for Research and Technological Development (CNPq) - grant -314045/2023-6. The authors would like to thank them for the financial support given to this research.

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