On the Computation of the Boundary Integral of Space–Time Deforming Finite Elements*

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Abstract

We present the integrated–by–parts version of the Time–Discontinuous Galerkin Least–Squares finite element formulation for the solution of the unsteady compressible Navier–Stokes equations in three dimension for problems involving moving boundary and interfaces. The deformation of the spatial domain is automatically taken into account writing the weak form of the problem over its space–time domain. The integration by parts in the three–dimensional spatial case is non–trivial, since one needs to apply the Gauss Theorem in a 4–D space–time continuum. We address the problem developing an application of the General Stokes' Theorem.

Introduction

The solution to fluid dynamic problems involving moving boundaries and interfaces, free surfaces or more in general deforming domains, has stimulated much research within the scientific community. The reason for this can be certainly identified in the fact that many problems of engineering interest are indeed moving boundary problems. Moreover, recent advances in computer hardware, and most notably the advent of scalable parallel computer architectures, has made compressible and incompressible flow problems within deforming domains tractable.

*Submitted to *Communications in Numerical Methods in Engineering.*

Several methods have been proposed in the literature for effectively treating deforming domain flow problems. The main difficulty that one must face when dealing with this class of problems, resides in the fact that the characterization of the motion of the boundaries is best accomplished within some form of Lagrangian description. On the other hand, a Lagrangian formulation of the flow problem at the interior of the domain usually causes serious difficulties, and an Eulerian description is certainly preferable. In order to overcome this empasse, the Arbitrary Lagrangian Eulerian (ALE) methods have been introduced [1] and successfully used in finite difference, finite volume and finite element approaches (see for example [2] for an application to the finite element method).

Recently, a very elegant solution to deforming domain flow problems has been proposed within the space–time finite element method [3][4][5]. The traditional approach to the finite element approximation of time–dependent problems relies on the discretization of the space dimension, which converts the PDE's in space and time into a set of ODE's in time only. The ODE's in time are then discretized by some form of differencing. An alternative approach is the space–time finite element method which performs a simultaneous discretization of the space and time dimensions. The finite element interpolating functions can be discontinuous in time, allowing the solution of the discrete problem to be performed one space–time slab at a time. The fact that the finite element statement of the problem is written over its space–time domain, automatically accounts for motions of the boundaries. In fact, finite element nodes lying on a moving boundary or interface move with it within the time step, creating space–time deformed finite elements. The Jacobian that relates the physical space–time coordinates with the local coordinates of the deformed finite elements, automatically accounts for the motion of the domain boundaries.

A part from the simplicity and beauty of the formulation, this approach has also the advantage of allowing a certain freedom in the motion of the mesh nodes within the domain. Therefore, various mesh motion or node repositioning techniques can be successfully used in conjunction with this methodology without the need of solution projection [5].

The space–time deforming element procedure has been always presented in the literature in its non–integrated–by–parts form [3][5][6][7]. However, it is well known that integration–by–parts performed on the weak form enhances the numerical properties of the formulation and leads to flux conservation. The non–integrated–by–parts form, in contrast, results in loss of conservation [8]. In this note, we develop an integrated–by–parts space–time deforming element procedure based on the stabilized Time–Discontinuous Galerkin Least–Squares (TDG/LS) formulation, and we shown how to compute the space–time boundary integral appearing in the formulation by resorting to the General Stokes' Theorem. The computation of the aforementioned boundary term is non–trivial in the three–dimensional spatial case, where the space–time boundary integral requires the computation of a space–time flux traversing a three–dimensional space–time region.

The work is organized as follows: a first section introduces the TDG/LS formulation for the compressible Navier–Stokes equations, in both integrated–by–parts and non–integrated–by–parts forms. A second section follows where the General Stokes' Theorem is employed for carrying out the computation of the resulting space–time boundary integral and explicit expressions for it are given in the three–dimensional spatial case.

Space–Time Finite Element Formulation of the Compressible Navier–Stokes Equations

The initial/boundary value problem for a viscous compressible fluid in n_{sd} dimensions can be expressed by means of the Navier–Stokes equations as

$$\boldsymbol{U}_{,t} + \boldsymbol{F}_{i,i} = \boldsymbol{F}^{d}_{i,i} + \boldsymbol{E}, \qquad (i = 1, \ldots, n_{sd}) \tag{1}$$

plus well posed initial and boundary conditions. In equation (1)

$$\boldsymbol{U} = \rho\,(1, u_1, u_2, u_3, e)$$

are the conservative variables,

$$\boldsymbol{F}_i = \rho\, u_i(1, u_1, u_2, u_3, e) + p\,(0, \delta_{1i}, \delta_{2i}, \delta_{3i}, u_i)$$

is the Euler flux,

$$\boldsymbol{F}^{d}_{i} = (0, \tau_{1i}, \tau_{2i}, \tau_{3i}, \tau_{ij} u_j) + (0, 0, 0, 0, -q_i)$$

is the diffusive flux, and

$$\boldsymbol{E} = \rho\,(0, b_1, b_2, b_3, b_i u_i + r)$$

is the source vector. In the previous expressions, ρ is the density, $\boldsymbol{u} = (u_1, u_2, u_3)$ is the velocity vector, e is the total energy, p is the pressure, δ_{ij} is the Kronecker delta, $\boldsymbol{\tau} = [\tau_{ij}]$ is the viscous stress tensor, $\boldsymbol{q} = (q_1, q_2, q_3)$

is the heat flux vector, $\boldsymbol{b} = (b_1, b_2, b_3)$ is the body force vector per unit mass and r is the heat supply per unit mass. The notation $a_{,i} = \partial a / \partial x_i$ is adopted in this work.

In n_{sd} dimensions, equations (1) can be given a more compact form defining the $n_{sd}+1$ vector field

$$\begin{aligned} \bar{\boldsymbol{F}} &= \left(\boldsymbol{U}, \boldsymbol{F}_j - \boldsymbol{F}_j^d\right) \quad (j = 1, \ldots, n_{sd}) \\ &= (\bar{\boldsymbol{F}}_i) \qquad\qquad\quad (i = 0, \ldots, n_{sd}) \end{aligned}$$

and introducing the divergence operator in $n_{sd}+1$ dimensions

$$\operatorname{div} \bar{\boldsymbol{F}} = \bar{\boldsymbol{F}}_{i,i} \quad (i = 0, \ldots, n_{sd}),$$

where $x_0 \equiv t$. The Navier–Stokes equations then simply write

$$\operatorname{div} \bar{\boldsymbol{F}} = \boldsymbol{E}. \tag{2}$$

Considering a partition $0 = t_0 < t_1 < \cdots < t_N = T$ of the time interval $I = (0, T)$, the space–time domain is divided in N space–time slabs. The slab Q_n corresponding to the n–th time interval $I_n = (t_n, t_{n+1})$ is a space–time region bounded by the evolving spatial domain $\mathcal{D}(t)$ of boundary $\Gamma(t)$ at times t_n and t_{n+1}, and by the space–time domain P_n described by $\Gamma(t)$ as it traverses the time interval I_n. A graphical representation of the space–time slab Q_n is depicted in Figure (1) for the case $n_{sd} = 2$.

The TDG/LS finite element method [8] is developed starting from the symmetric form of the Euler equations expressed in terms of the entropy variables $\boldsymbol{V}$. A least–squares operator and a discontinuity capturing term are added to the formulation for improving stability without sacrificing accuracy.

Choosing $\boldsymbol{W}^h$ and $\boldsymbol{V}^h$ as suitable spaces for test and trial functions[§], the TDG/LS finite element method takes the basic form

$$\begin{aligned} &\int_{Q_n} \boldsymbol{W}^h \cdot \left(\operatorname{div} \bar{\boldsymbol{F}}(\boldsymbol{V}^h) - \boldsymbol{E}(\boldsymbol{V}^h)\right) \mathrm{d}Q \\ &+ \int_{\mathcal{D}(t_n^+)} \boldsymbol{W}^h \cdot \left(\boldsymbol{U}(\boldsymbol{V}^{h^+}) - \boldsymbol{U}(\boldsymbol{V}^{h^-})\right) \mathrm{d}\mathcal{D} \\ &+ \sum_{e=1}^{(n_{el})_n} \int_{Q_n^e} \left(\mathcal{L}\boldsymbol{W}^h\right) \cdot \tau \left(\mathcal{L}\boldsymbol{V}^h\right) \mathrm{d}Q \end{aligned}$$

[§]We remark that, in order to avoid subparametric representations, the temporal discretization must be at least liner–in–time for moving boundary problems.

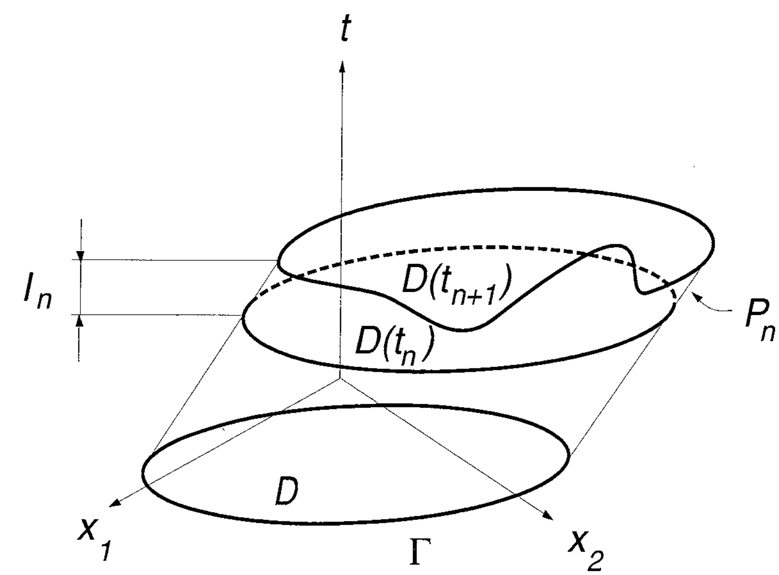

Figure 1: A deforming space–time slab in 2–D space.

$$+\sum_{e=1}^{(n_{el})_n}\int_{Q_n^e}\nu^h\hat{\nabla}_\xi \boldsymbol{W}^h\cdot\mathrm{diag}\,[\tilde{\boldsymbol{A}}_0]\hat{\nabla}_\xi \boldsymbol{V}^h\,\mathrm{d}Q=0, \tag{3}$$

where the first term is the Galerkin term, the second is a jump term that weakly enforces the initial conditions for the space–time slab, and the third and fourth terms are respectively the Least–Squares stabilization τ term and Discontinuity Capturing ν^h term. $\tilde{\boldsymbol{A}}_0=\partial\boldsymbol{U}/\partial\boldsymbol{V}$ is the metric tensor of the transformation from conservation to entropy variables. Refer to [8] for additional details on the TDG/LS finite element formulation.

Equation (3) results in loss of conservation of fluxes, which is on the contrary achieved under inexact quadrature by its integrated–by–parts form [8]

$$\int_{Q_n}\left(-\mathrm{grad}\,\boldsymbol{W}^h\cdot\bar{\boldsymbol{F}}(\boldsymbol{V}^h)+\boldsymbol{W}^h\cdot\boldsymbol{E}(\boldsymbol{V}^h)\right)\mathrm{d}Q$$

$$+\int_{\mathcal{D}(t_{n+1})}\boldsymbol{W}^{h^-}\cdot\boldsymbol{U}(\boldsymbol{V}^{h^-})\,\mathrm{d}\mathcal{D}-\int_{\mathcal{D}(t_n)}\boldsymbol{W}^{h^+}\cdot\boldsymbol{U}(\boldsymbol{V}^{h^-})\,\mathrm{d}\mathcal{D}$$

$$+\int_{P_n}\boldsymbol{W}^h\,\bar{\boldsymbol{F}}(\boldsymbol{V}^h)\cdot\mathrm{d}\boldsymbol{P}$$

$$+\sum_{e=1}^{(n_{el})_n}\int_{Q_n^e}\left(\mathcal{L}\boldsymbol{W}^h\right)\cdot\tau\left(\mathcal{L}\boldsymbol{V}^h\right)\,\mathrm{d}Q$$

$$+\sum_{e=1}^{(n_{el})_n}\int_{Q_n^e}\nu^h\hat{\nabla}_\xi\boldsymbol{W}^h\cdot\mathrm{diag}\,[\tilde{\boldsymbol{A}}_0]\hat{\nabla}_\xi\boldsymbol{V}^h\,\mathrm{d}Q=0, \tag{4}$$

where grad is the gradient operator in $n_{sd}+1$ dimensions and $\mathrm{d}\boldsymbol{P}$ is an oriented infinitesimal portion of the space–time boundary P_n. The first term results from the integration–by–parts of the Galerkin integral, the second from the combination of the jump term with the time flux that flows through the time surfaces $\mathcal{D}(t_n)$ and $\mathcal{D}(t_{n+1})$, the third term is a boundary integral generated by the space–time flux through the space–time boundaries P_n of the slab, while the last two terms keep the same meaning as in (3).

In the following, we give eplicit expressions for computing the boundary integral term in (4).

Application of the General Stokes' Theorem to Space–Time Deforming Finite Elements

The computation of the boundary integral $\int_{P_n}\boldsymbol{W}^h\,\bar{\boldsymbol{F}}(\boldsymbol{V}^h)\cdot\mathrm{d}\boldsymbol{P}$ can be performed resorting to the General Stokes' Theorem: Let Q be an open subset of R^n, ω a $(p-1)$–form on Q, and C a singular p–chain on Q. Then

$$\int_{\partial C}\omega=\int_C\mathrm{d}\,\omega. \tag{5}$$

See [9] for additional details.

In the following we fix our attention to the case $n_{sd}=3$, therefore in this case $C:I^4\to R^4$ is a singular 4–cube. Considering the special topology of the space–time slab Q, it is convenient to formally define the boundary of C as the singular 3–chain $\partial C=\partial C_{P_n}+\partial C_{\mathcal{D}_n}+\partial C_{\mathcal{D}_{n+1}}$.

In order to compute the boundary integral in question, let us consider the 3–form

$$\omega=\bar{\boldsymbol{F}}_0\,\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3-\bar{\boldsymbol{F}}_1\,\mathrm{d}x_0\mathrm{d}x_2\mathrm{d}x_3+\bar{\boldsymbol{F}}_2\,\mathrm{d}x_0\mathrm{d}x_1\mathrm{d}x_3-\bar{\boldsymbol{F}}_3\,\mathrm{d}x_0\mathrm{d}x_1\mathrm{d}x_2 \tag{6}$$

associated with the 4–D vector field $\bar{\boldsymbol{F}}=(\bar{\boldsymbol{F}}_i)$, $(i=0,\ldots,3)$. The terms $\mathrm{d}x_i\mathrm{d}x_j$ are the product of the 1–form $\mathrm{d}x_i$ with the 1–form $\mathrm{d}x_j$, and enjoy the well know property

$$\mathrm{d}x_i\mathrm{d}x_j=-\mathrm{d}x_j\mathrm{d}x_i\quad\forall\quad i,j=0,\ldots,3$$

which explains the alternating signs in (6).

div $\bar{\boldsymbol{F}}$ is then the function corresponding to the exterior differential of the 3–form ω associated with $\bar{\boldsymbol{F}}$, i.e.

$$\mathrm{d}\omega = \mathrm{div}\bar{\boldsymbol{F}}\, \mathrm{d}x_0 \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3.$$

By the General Stokes' Theorem, we consequently have for each space–time slab

$$\int_{Q_n} \mathrm{div}\bar{\boldsymbol{F}}\, \mathrm{d}Q = \int_{\partial C} \omega. \tag{7}$$

The computation of the time fluxes traversing $\partial C_{\mathcal{D}_n}$ and $\partial C_{\mathcal{D}_{n+1}}$ associated respectively with $\mathcal{D}(t_n)$ and $\mathcal{D}(t_{n+1})$ is straightforward, and the resulting terms combine themselves with the jump terms in (3) producing the second term of (4).

From (7), the computation of the space–time fluxes that traverse the 3–D space–time region P_n is immediate. Introducing the local space–time boundary element coordinates ξ_0, ξ_1 and ξ_2, from (6) and (7) we easily obtain that

$$\int_{\partial C_{P_n}} \omega = \int_{\xi_0,\xi_1,\xi_2=0,1} \boldsymbol{P}\, \mathrm{d}\xi_0 \mathrm{d}\xi_1 \mathrm{d}\xi_2,$$

having defined $\boldsymbol{P} = (P_i)$ $(i = 0, \ldots, 3)$ as

$$\begin{aligned}
P_0 &= -(x_{2,1}x_{3,2} - x_{2,2}x_{3,1})\, x_{1,0} - (x_{1,2}x_{3,1} - x_{1,1}x_{3,2})\, x_{2,0} - (x_{1,1}x_{2,2} - x_{1,2}x_{2,1})\, x_{3,0}, \\
P_1 &= (x_{2,1}x_{3,2} - x_{2,2}x_{3,1})\, x_{0,0} + (x_{2,2}x_{3,0} - x_{2,0}x_{3,2})\, x_{0,1} + (x_{2,0}x_{3,1} - x_{2,1}x_{3,0})\, x_{0,2}, \\
P_2 &= (x_{1,2}x_{3,1} - x_{1,1}x_{3,2})\, x_{0,0} + (x_{1,0}x_{3,2} - x_{1,2}x_{3,0})\, x_{0,1} + (x_{1,1}x_{3,0} - x_{1,0}x_{3,1})\, x_{0,2}, \\
P_3 &= (x_{1,1}x_{2,2} - x_{1,2}x_{2,1})\, x_{0,0} + (x_{1,2}x_{2,0} - x_{1,0}x_{2,2})\, x_{0,1} + (x_{1,0}x_{2,1} - x_{1,1}x_{2,0})\, x_{0,2}.
\end{aligned}$$

This expression allows the computation of the boundary integral in the most general case of an arbitrary domain in $n_{sd}+1$ space. However in the specific case here considered, from the definition of the space–time slab given previously we clearly have that $x_{0,1} = 0$ and $x_{0,2} = 0$. In this case the expression for P_1, P_2 and P_3 simplifies to

$$\begin{aligned}
P_1 &= (x_{2,1}x_{3,2} - x_{2,2}x_{3,1})\, x_{0,0}, \\
P_2 &= (x_{1,2}x_{3,1} - x_{1,1}x_{3,2})\, x_{0,0}, \\
P_3 &= (x_{1,1}x_{2,2} - x_{1,2}x_{2,1})\, x_{0,0}.
\end{aligned}$$

These are nothing else than the familiar components of the normal to a surface, multiplied by the time step $\Delta t_n = t_{n+1} - t_n = x_{0,0}$. Letting $\boldsymbol{n} =$

(n_1, n_2, n_3) be the normal to the spatial boundary, the term P_0 can then be written as $P_0 = -\boldsymbol{n} \cdot \boldsymbol{v}\, \Delta t_n$, where $\boldsymbol{v} = \boldsymbol{x}_{,t}$ is the velocity of the moving boundary.

This expression represents a convenient way of computing the boundary integral term in equation (4) as

$$\int_{P_n} \boldsymbol{W}^h\, \bar{\boldsymbol{F}}(\boldsymbol{V}^h) \cdot \mathrm{d}\boldsymbol{P} =$$

$$\Delta t_n \int_{\xi_0,\xi_1,\xi_2=0,1} \boldsymbol{W}^h \left(-\boldsymbol{U}(\boldsymbol{V}^h)\, \boldsymbol{n} \cdot \boldsymbol{v} + \boldsymbol{F}_i(\boldsymbol{V}^h)\, n_i\right) \mathrm{d}\xi_0 \mathrm{d}\xi_1 \mathrm{d}\xi_2 =$$

$$\Delta t_n \int_{\xi_0,\xi_1,\xi_2=0,1} \boldsymbol{W}^h \left(\boldsymbol{U}(\boldsymbol{V}^h)\, \boldsymbol{n}\cdot(\boldsymbol{u}-\boldsymbol{v}) + p\,(0, n_1, n_2, n_3, \boldsymbol{u}\cdot\boldsymbol{n})\right) \mathrm{d}\xi_0 \mathrm{d}\xi_1 \mathrm{d}\xi_2. \quad (8)$$

Conclusions

In this note we have introduced the integrated–by–parts form of the space–time deforming element formulation for dealing with moving boundary problems in the context of the compressible Navier–Stokes equations. By resorting to the General Stokes' Theorem, we have given explicit expressions for the computation of the resulting space–time boundary integrals. It is worth stressing the fact that the same ideas can be readily applied to other deforming domain problems in the context of the space–time finite element technique.

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