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Introduction to the Fractional Step Method

by CTTC

Abstract —
This document is concerned with techniques for the solution of the unsteady, incompressible Navier-Stokes equations in primitive variables. In particular, we focus our attention to the fractional step (or projection) method, first introduced in the pioneering works by Chorin [1] and Temam [2]. The main mathematical ideas behind the method are briefly discussed. Finally, the algorithm is concretised for a fully explicit second-order accurate formulation.

1. Introduction

Despite all the inherent difficulties[1], the fractional step methods has become a very popular technique for solving the incompressible Navier-Stokes equations. The main reasons for this success are basically:

- Better performance[2] than other methods such as SIMPLE-like [4, 5] algorithms.
- Code simplicity.

Fractional step methods are also referred to as projection methods because the system of equations given can be interpreted as a projection into a divergence-free velocity space. The *predictor velocity*, is an approximate solution of the momentum equations, but because the predictor velocity is obtained with no pressure gradient contribution it cannot satisfy the incompressibility constraint at the next time level. Them, the Poisson equation determines the minimum perturbation that will make the predictor velocity incompressible.

The rest of the document is organised as follows. In section 2, the incompressible Navier-Stokes equations are presented. In section 3, a short theoretical background for the fractional step method is given. The gradient pressure term of the momentum equation is viewed as a projector into a divergence-free space. To do so, the Helmholtz-Hodge decomposition theorem outlined in the Appendix A plays an important role. Finally, the final form of the time-integration algorithm is presented in the section 4.

[1] There are still some controversy related with the temporal accuracy of the method and some debate about how the boundary conditions should be specified (see [3], for a review).

[2] Specially for fully-explicit or semi-implicit formulations.

2. Incompressible Navier-Stokes equations

We consider the simulation of incompressible flows of Newtonian fluids. Under these assumptions[3], the dimensionless governing equations in primitive variables are

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\,\boldsymbol{u} = \frac{1}{Re}\Delta \boldsymbol{u} - \nabla p \tag{1}$$

$$\nabla \cdot \boldsymbol{u} = 0 \tag{2}$$

where Re is the dimensionless Reynolds number defined as

$$Re = \frac{\rho V_0 L}{\mu} \tag{3}$$

where ρ and μ are the density and the dynamic viscosity of the working fluid. L and V_0 are the characteristic length and velocity, respectively.

Since Claude Navier[4] (1822) and George Stokes[5] (1845) derived this set of partial differential equations, they have attracted the interests of many physicists, engineers and mathematicians. High accurate numerical solutions over the past two decades [6, 7, 8, 9, 10, 11] have evidenced that these equations form an excellent mathematical model for turbulent flow. However, more than one and a half century later our understanding of them remains minimal. For instance, the existence and uniqueness of general solutions remains an open question[6].

3. Application of the Helmholtz-Hodge decomposition theorem to the incompressible Navier-Stokes equations. Role of the pressure.

In this section, the Helmholtz-Hodge decomposition theorem (see Appendix A, for details) is applied to the incompressible Navier-Stokes equations. The results here obtained will help us to better elucidate the role of the pressure field.

Let $\Pi(\cdot)$ be a projector operator. It projects any vector field onto a divergence-free space[7]

$$\nabla \cdot \Pi(\boldsymbol{a}) = 0 \tag{6}$$

Now, taking the Navier-Stokes equations and applying the projector operator

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[3] Actually, more assumptions are needed to formally derive the incompressible Navier-Stokes. However, they are not relevant in our context.

[4] A french engineer specialist in road and bridge building. He was the first to arrive at the proper form for NS-equations although the reasonings he used were not formally correct.

[5] Irish mathematician and physicist. He was the first to formally derived the NS-equations.

[6] Actually, this is one of the seven 1$ million dollar "Millennium Prize Problems" proposed by the Clay Mathematics Institute of Cambridge, Massachusetts (CMI) on May 2000. For more information you can visit: http://www.claymath.org/millennium/

[7] Note that any incompressible field remains unchanged by the action of the projector operator $\Pi(\cdot)$

$$\text{if} \quad \nabla \cdot \boldsymbol{a} = 0 \quad \Longrightarrow \quad \Pi(\boldsymbol{a}) = \boldsymbol{a} \tag{4}$$

moreover, applying the projector operator, $\Pi(\cdot)$, to (A.1) yields to the following property

$$\Pi(\nabla\varphi) = \Pi(\boldsymbol{w}) - \Pi(\boldsymbol{a}) = \boldsymbol{a} - \boldsymbol{a} = 0 \tag{5}$$

$$\Pi\left(\frac{\partial \boldsymbol{u}}{\partial t}+\nabla p\right)=\Pi\left(-\left(\boldsymbol{u}\cdot\nabla\right)\boldsymbol{u}+\frac{1}{Re}\Delta\boldsymbol{u}\right) \tag{7}$$

Since the velocity field is incompressible the transient term remains unchanged (see Eq. 4) when projected

$$\Pi\left(\frac{\partial \boldsymbol{u}}{\partial t}\right)=\frac{\partial \boldsymbol{u}}{\partial t} \tag{8}$$

whereas the projection of the pressure gradient vanishes (see Eq. 5)

$$\Pi\left(\nabla p\right)=0 \tag{9}$$

Therefore, Navier-Stokes equations can be splitted in two parts: a divergence-free vector and a gradient of an scalar field[8]

$$\frac{\partial \boldsymbol{u}}{\partial t} = \Pi\left(-\left(\boldsymbol{u}\cdot\nabla\right)\boldsymbol{u}+\frac{1}{Re}\Delta\boldsymbol{u}\right) \tag{12}$$

$$\nabla p = -\left(\boldsymbol{u}\cdot\nabla\right)\boldsymbol{u}+\frac{1}{Re}\Delta\boldsymbol{u}-\Pi\left(-\left(\boldsymbol{u}\cdot\nabla\right)\boldsymbol{u}+\frac{1}{Re}\Delta\boldsymbol{u}\right) \tag{13}$$

The Helmholtz-Hodge decomposition theorem ensures that this decomposition is **unique!**

Finally, applying the divergence operator to (13) and using projector definition (6) leads to a Poisson equation for pressure

$$\Delta p=\nabla\cdot\left(-\left(\boldsymbol{u}\cdot\nabla\right)\boldsymbol{u}+\frac{1}{Re}\Delta\boldsymbol{u}\right) \tag{14}$$

$\Longrightarrow$ Therefore, for *incompressible flows* the role of the *pressure gradient* is to *project* the vector field $\boldsymbol{R}\left(\boldsymbol{u}\right)$ into a divergence-free space.

[8]Note that in the continuous formulation the viscous term is also incompressible. Recalling identity (B.12) and the incompressibility condition ($\nabla\cdot\boldsymbol{u}=0$), the viscous terms can be rewritten in rotational form

$$\Delta\boldsymbol{u}=\nabla\left(\nabla\cdot\boldsymbol{u}\right)-\nabla\times\left(\nabla\times\boldsymbol{u}\right)=-\nabla\times\left(\nabla\times\boldsymbol{u}\right) \tag{10}$$

then, applying the divergence and using the identity (B.2)

$$\nabla\cdot\left(\Delta\boldsymbol{u}\right)=-\nabla\cdot\left(\nabla\times\left(\nabla\times\boldsymbol{u}\right)\right)=0 \tag{11}$$

However, at a discrete level, in general, the divergence of the viscous terms would not exactly vanish. The sources of errors are twofold:

- If the operators are not consistently discretized the identity (B.2) would not be exactly satisfied in a discrete sense.
- It is assumed that incompressibility constraint is exactly accomplished (10). This is not true in general.

First source of errors can be eliminated using the support-operator idea (use one operator to generate the others) consistently [12, 13, 14]. Second source may be eliminated ensuring that the velocity field is exactly incompressible. Anyhow, in order to avoid round-off errors to accumulate, it is always preferable to treat viscous term not assuming to be incompressible. Thus, for the aforementioned reasons, we prefer to adopt the idea that the viscous term also need to be projected.

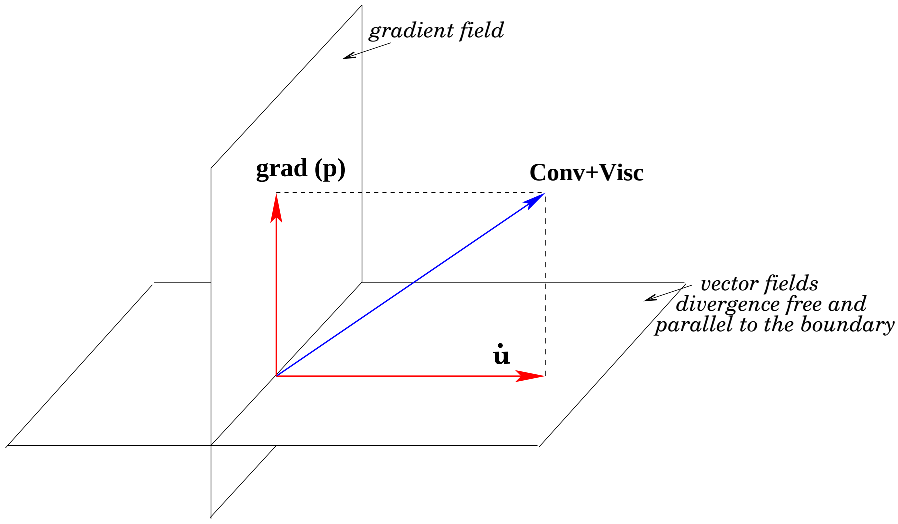

Figure 1: Convective + Viscous term vector field unique decomposition.

4. Time-integration method

The final form of the fractional step method would depend on the time-integration method chosen. Here, for the sake of clarity, we propose to use a fully explicit time integration scheme. In order to simplify the notation, momentum equation can be rewritten as

$$\frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{R}\left(\boldsymbol{u}\right) - \nabla p \tag{15}$$

where $\boldsymbol{R}\left(\boldsymbol{u}\right)$ stands for the convective and diffusive terms

$$\boldsymbol{R}\left(\boldsymbol{u}\right) \equiv -\left(\boldsymbol{u}\cdot\nabla\right)\boldsymbol{u} + \frac{1}{Re}\Delta\boldsymbol{u} \tag{16}$$

For the temporal discretization, a central difference scheme is used for the time derivative term,

$$\left.\frac{\partial \boldsymbol{u}}{\partial t}\right|^{n+1/2} \approx \frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^{n}}{\Delta t} + \mathcal{O}\left(\Delta t^2\right) \tag{17}$$

a fully explicit second-order Adams-Bashforth scheme for $\boldsymbol{R}\left(\boldsymbol{u}\right)$

$$\boldsymbol{R}^{n+1/2}\left(\boldsymbol{u}\right) \approx \frac{3}{2}\boldsymbol{R}\left(\boldsymbol{u}^{n}\right) - \frac{1}{2}\boldsymbol{R}\left(\boldsymbol{u}^{n-1}\right) + \mathcal{O}\left(\Delta t^2, \Delta x^m\right) \tag{18}$$

and a first-order backward Euler scheme for the pressure-gradient term. Incompressibility constraint is treated implicitly. Thus, we obtain the semi-discretized Navier-Stokes equations

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^{n}}{\Delta t} = \frac{3}{2}\boldsymbol{R}\left(\boldsymbol{u}^{n}\right) - \frac{1}{2}\boldsymbol{R}\left(\boldsymbol{u}^{n-1}\right) - \nabla p^{n+1} \tag{19}$$

$$\nabla\cdot\boldsymbol{u}^{n+1} = 0 \tag{20}$$

To solve the velocity-pressure coupling we use a classical fractional step projection method [1, 2, 15]. In the projection methods, solutions of the unsteady Navier-Stokes equations are obtained by first time-advancing the velocity field $\boldsymbol{u}$ without regard for its incompressibility constraint (20). Then, the pressure gradient forces (projects) the predictor velocity field to be incompressible ($\nabla \cdot \boldsymbol{u}^{n+1} = 0$). This projection is derived from the well-known Helmholtz-Hodge vector decomposition theorem (see Appendix A), whereby the predictor velocity $\boldsymbol{u}^p$ can be uniquely decomposed into a divergence-free vector, $\boldsymbol{u}^{n+1}$, and the gradient of a scalar field, $\nabla\tilde{p}$. This decomposition is written as

$$\boldsymbol{u}^p = \boldsymbol{u}^{n+1} + \nabla\tilde{p} \tag{21}$$

where the predictor velocity $\boldsymbol{u}^p$ is given by

$$\boldsymbol{u}^p = \boldsymbol{u}^n + \Delta t \left(\frac{3}{2}\boldsymbol{R}\left(\boldsymbol{u}^n\right) - \frac{1}{2}\boldsymbol{R}\left(\boldsymbol{u}^{n-1}\right) \right) \tag{22}$$

and the pseudo-pressure is $\tilde{p} = \Delta t\, p^{n+1}$. Taking the divergence of (21) yields a Poisson equation for $\tilde{p}$

$$\nabla \cdot \boldsymbol{u}^p = \nabla \cdot \boldsymbol{u}^{n+1} + \nabla \cdot (\nabla\tilde{p}) \longrightarrow \Delta\tilde{p} = \nabla \cdot \boldsymbol{u}^p \tag{23}$$

Once the solution is obtained, $\boldsymbol{u}^{n+1}$ results from the correction

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^p - \nabla\tilde{p} \tag{24}$$

Therefore, the algorithm for the integration of each time step is

1. Evaluate $\boldsymbol{R}\left(\boldsymbol{u}^n\right)$.
2. Evaluate $\boldsymbol{u}^p$ from Eq. (22).
3. Evaluate $\nabla \cdot \boldsymbol{u}^p$ and solve the discrete Poisson (23) equation.
4. Obtain the new velocity field with Eq. (24).

4.1. Determination of Δt

Due to stability reasons explicit temporal schemes introduce severe restrictions on the time step, while implicit discretization would improve the overall stability. The final performance of time-integration method would be case dependant: for instance, the use of implicit methods in DNS/LES of turbulent flows the computational costs are rather high compared to those of explicit methods. This is because of the underlying restrictions to time step that are required to fully resolve all temporal scales in the Navier-Stokes equations [7, 16, 12]. On the other hand, implicit methods are very convenient for pseudo-transient simulations of laminar steady flows [4]. Here, we have only considered explicit method in the view of formulation simplicity.

Therefore, in our case, the time-step, Δt, must be bounded by the CFL condition [17] given by

$$\Delta t \left(\frac{|u_i|}{\Delta x_i} \right)_{max} \leq C_{\text{conv}} \tag{25}$$

$$\Delta t \left(\frac{\nu}{\Delta x_i^2} \right)_{max} \leq C_{\text{visc}} \tag{26}$$

where the bounding values C_{conv} are C_{visc} must be smaller than unity. In our case, we will follow the recommendations given by [18] using values $C_{\text{conv}} = 0.35$ and $C_{\text{visc}} = 0.2$, respectively.

Note that, since the mesh would remain constant during all the simulation, only the CFL-condition for the convective term (25) has to be recomputed each time-step.

4.2. Solution of Poisson equation

Since the formulation is fully explicit, the only system to be solved is the pressure Poisson equation (23). Thus, in our case, the efficient solution of the Poisson equation would be a critical aspect.

A Theoretical background: the Helmholtz-Hodge theorem

The Helmholtz-Hodge decomposition theorem plays a basic role in the theory of the numerical approximation of a variety of physical models. Fractional step (or projection) methods applied to the numerical solution of the incompressible Navier-Stokes equations is one of them.

A "slightly" simplified version of the Helmholtz-Hodge theorem states:

Theorem 1. *A given vector field $\boldsymbol{w}$, defined in a bounded domain Ω with smooth boundary $\partial\Omega$, is uniquely decomposed in a pure gradient field and a divergence-free vector parallel to $\partial\Omega$*

$$\boldsymbol{w} = \boldsymbol{a} + \nabla\varphi \tag{A.1}$$

where

$$\begin{aligned} \nabla \cdot \boldsymbol{a} &= 0 \quad \boldsymbol{a} \in \Omega & \text{(A.2)} \\ \boldsymbol{a} \cdot \boldsymbol{n} &= 0 \quad \boldsymbol{a} \in \partial\Omega & \text{(A.3)} \end{aligned}$$

Proof. Recalling vector identity (B.5) and considering that $\boldsymbol{a}$ is divergence-free (A.2) follows

$$\nabla \cdot (\varphi \boldsymbol{a}) = (\nabla\varphi) \cdot \boldsymbol{a} \tag{A.4}$$

Integrating previous expression over the domain Ω and applying the Gauss divergence theorem leads

$$\begin{aligned} \int_{\Omega} (\nabla\varphi) \cdot \boldsymbol{a} d\Omega &= \int_{\Omega} \nabla \cdot (\varphi \boldsymbol{a})\, d\Omega & \text{(A.5)} \\ &= \int_{\partial\Omega} (\varphi \boldsymbol{a} \cdot \boldsymbol{n})\, dS & \text{(A.6)} \end{aligned}$$

Boundary integral vanishes if $\boldsymbol{a}$ satisfies the prescribed condition (A.3). Therefore, the orthogonality[9] between vector field $\boldsymbol{a}$ and $\nabla\varphi$ is proved

$$\int_{\Omega} (\nabla\varphi) \cdot \boldsymbol{a} d\Omega = 0 \tag{A.8}$$

From previous expression, it is easy to prove the unicity of the decomposition. First, we assume two different decompositions exist

$$\boldsymbol{w} = \boldsymbol{a}_1 + \nabla\varphi_1 = \boldsymbol{a}_2 + \nabla\varphi_2 \tag{A.9}$$

rearraging terms

$$\boldsymbol{a}_1 - \boldsymbol{a}_2 + \nabla(\varphi_1 - \varphi_2) = 0 \tag{A.10}$$

[9] For the standard inner product of two vector fields, $\boldsymbol{a}$ and $\boldsymbol{b}$, defined as follows:

$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_{\Omega} \boldsymbol{a} \cdot \boldsymbol{b} d\Omega \tag{A.7}$$

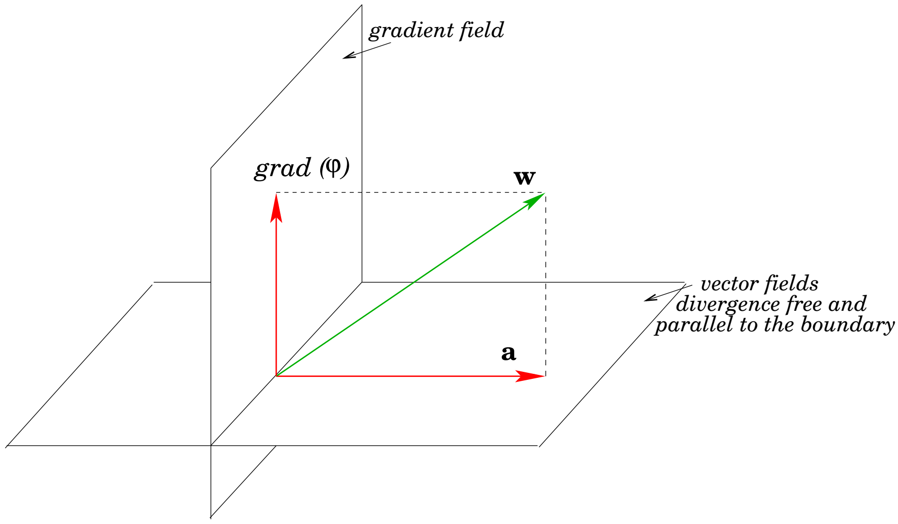

Figure 2: Vector field unique decomposition.

Now, the scalar product of previous expression by vector $(\boldsymbol{a}_1 - \boldsymbol{a}_2)$ and the orthogonality relation (A.8) leads

$$\begin{aligned} 0 &= \int_\Omega \|\boldsymbol{a}_1 - \boldsymbol{a}_2\|^2 + (\boldsymbol{a}_1 - \boldsymbol{a}_2) \cdot \nabla (\varphi_1 - \varphi_2)\, d\Omega \\ &= \int_\Omega \|\boldsymbol{a}_1 - \boldsymbol{a}_2\|^2\, d\Omega \end{aligned} \tag{A.11}$$

Finally, from expressions (A.10) and (A.11), it follows the unicity of the decomposition (A.1)

$$\boldsymbol{a}_1 = \boldsymbol{a}_2 \tag{A.12}$$

$$\nabla\varphi_1 = \nabla\varphi_2 \implies \varphi_1 = \varphi_2 + constant \tag{A.13}$$

$\square$

It should be noted that the unicity of the decomposition (A.1) *do not imply*, as stated by Eq.(A.13), that the scalar field φ be uniquely determined.

B Useful formulas of vector analysis

$$
\begin{aligned}
\nabla\cdot\nabla\boldsymbol{a} &= \Delta\boldsymbol{a}=\nabla^2\boldsymbol{a} && \text{(B.1)}\\
\nabla\cdot(\nabla\times\boldsymbol{a}) &= 0 && \text{(B.2)}\\
\nabla\times(\nabla\varphi) &= 0 && \text{(B.3)}\\
\nabla\cdot((\nabla\boldsymbol{a})^*) &= \nabla(\nabla\cdot\boldsymbol{a}) && \text{(B.4)}\\
\nabla\cdot(\varphi\boldsymbol{a}) &= (\nabla\varphi)\cdot\boldsymbol{a}+\varphi(\nabla\cdot\boldsymbol{a}) && \text{(B.5)}\\
\nabla\cdot(\mathsf{T}\cdot\boldsymbol{a}) &= (\nabla\boldsymbol{a}):\mathsf{T}+\boldsymbol{a}\cdot(\nabla\cdot\mathsf{T}) && \text{(B.6)}\\
\nabla\cdot(\boldsymbol{a}\cdot\mathsf{T}) &= (\nabla\boldsymbol{a}):\mathsf{T}+\boldsymbol{a}\cdot(\nabla\cdot\mathsf{T}) \qquad \text{if } \mathsf{T}=\mathsf{T}^* && \text{(B.7)}\\
\nabla\times(\varphi\boldsymbol{a}) &= (\nabla\varphi)\times\boldsymbol{a}+\varphi(\nabla\times\boldsymbol{a}) && \text{(B.8)}\\
\nabla(\boldsymbol{a}\cdot\boldsymbol{b}) &= (\boldsymbol{a}\cdot\nabla)\boldsymbol{b}+(\boldsymbol{b}\cdot\nabla)\boldsymbol{a}+\boldsymbol{a}\times(\nabla\times\boldsymbol{b})+\boldsymbol{b}\times(\nabla\times\boldsymbol{a}) && \text{(B.9)}\\
\nabla\cdot(\boldsymbol{a}\times\boldsymbol{b}) &= \boldsymbol{b}\cdot(\nabla\times\boldsymbol{a})-\boldsymbol{a}\cdot(\nabla\times\boldsymbol{b}) && \text{(B.10)}\\
\nabla\times(\boldsymbol{a}\times\boldsymbol{b}) &= \boldsymbol{a}(\nabla\cdot\boldsymbol{b})-\boldsymbol{b}(\nabla\cdot\boldsymbol{a})+(\boldsymbol{b}\cdot\nabla)\boldsymbol{a}-(\boldsymbol{a}\cdot\nabla)\boldsymbol{b} && \text{(B.11)}\\
\nabla\times(\nabla\times\boldsymbol{a}) &= \nabla(\nabla\cdot\boldsymbol{a})-\Delta\boldsymbol{a} && \text{(B.12)}\\
(\boldsymbol{a}\cdot\nabla)\boldsymbol{a} &= \frac{1}{2}\nabla|\boldsymbol{a}|^2+(\nabla\times\boldsymbol{a})\times\boldsymbol{a} && \text{(B.13)}\\
\boldsymbol{a}\times(\nabla\times\boldsymbol{b}) &= (\nabla\boldsymbol{b})\cdot\boldsymbol{a}-\boldsymbol{a}\cdot(\nabla\boldsymbol{b}) && \text{(B.14)}\\
\nabla\times(\nabla\cdot(\nabla\boldsymbol{a})) &= \nabla\cdot(\nabla(\nabla\times\boldsymbol{a})) && \text{(B.15)}
\end{aligned}
$$

where φ is an scalar, $\boldsymbol{a}$ and $\boldsymbol{b}$ are vectors and T is a tensor. The following four vector equations are also often useful

$$
\begin{aligned}
\boldsymbol{a}\cdot(\boldsymbol{b}\times\boldsymbol{c}) &= \boldsymbol{b}\cdot(\boldsymbol{c}\times\boldsymbol{a})=\boldsymbol{c}\cdot(\boldsymbol{a}\times\boldsymbol{b}) && \text{(B.16)}\\
\boldsymbol{a}\times(\boldsymbol{b}\times\boldsymbol{c}) &= (\boldsymbol{a}\cdot\boldsymbol{c})\boldsymbol{b}-(\boldsymbol{a}\cdot\boldsymbol{b})\boldsymbol{c} && \text{(B.17)}\\
(\boldsymbol{a}\times\boldsymbol{b})\cdot(\boldsymbol{c}\times\boldsymbol{d}) &= \boldsymbol{a}\cdot[\boldsymbol{b}\times(\boldsymbol{c}\times\boldsymbol{d})]=(\boldsymbol{a}\cdot\boldsymbol{c})(\boldsymbol{b}\cdot\boldsymbol{d})-(\boldsymbol{a}\cdot\boldsymbol{d})(\boldsymbol{b}\cdot\boldsymbol{c}) && \text{(B.18)}\\
(\boldsymbol{a}\times\boldsymbol{b})\times(\boldsymbol{c}\times\boldsymbol{a}) &= (\boldsymbol{a}\times\boldsymbol{b}\cdot\boldsymbol{d})\boldsymbol{c}-(\boldsymbol{a}\times\boldsymbol{b}\cdot\boldsymbol{c})\boldsymbol{d} && \text{(B.19)}
\end{aligned}
$$

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