

051176 - Computational Techniques for Thermochemical Propulsion Master of Science in Aeronautical Engineering

Boundary Treatment in the FV Method

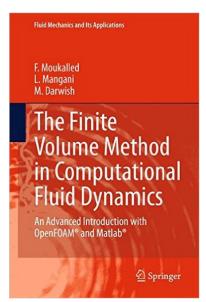
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Bibliography





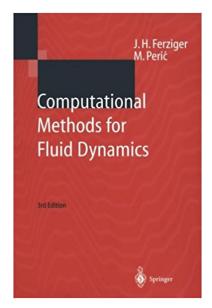
Some figures in this slides are taken from the reference text book:

F. Moukalled, L. Mangani, M. Darwish. "The Finite Volume Method in Computational Fluid Dynamics", Springer International Publishing Switzerland 2016.

Prof. Marwan Darwish is greatly acknowledged for sharing the images from his book and for allowing to include them in this course's material.

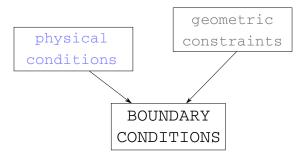
Bibliography





Ferziger, Joel H., Peric, Milovan. "Computational Methods for Fluid Dynamics", Third Edition, Springer 2002.

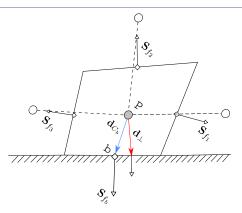




It is important to differentiate between physical conditions, geometric constraints, and boundary conditions at a domain boundary.

- "inlet", "outlet", or "wall" represent a physical condition;
- "symmetry" and "periodicity" represent geometric constraints;
- a boundary condition refers to the set of equations used along a domain boundary to obtain a specific solution to the problem.

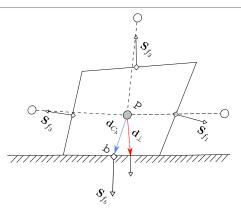




Each CV provides one algebraic equation. Volume integrals are calculated in the same way for every CV, but fluxes through CV faces coinciding with the domain boundary require special treatment.

These boundary fluxes must either be known, or be expressed as a combination of interior values and boundary data. Since they do not give additional equations, they should not introduce additional unknowns. Since there are no nodes outside the boundary, these approximations must be based on one-sided differences or extrapolations.

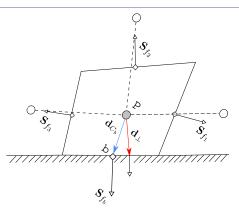




In the FVM, the discretization process starts by integrating the governing equations over the CVs. With the divergence theorem, the volume integrals of the convection and diffusion terms are transformed into surface integrals:

$$a_P \phi_P + \sum_f a_{P,f} \phi_{P,f} = \boldsymbol{b}_C$$





In the segregated pressure-based algorithms, governing equations are solved sequentially. The final algebraic form of any governing equation is written as:

$$a_P \phi_P + \underbrace{\sum_f^{n_f-1} a_{P_f} \phi_{P_f}}_{flux \text{ from the boundary}} = \boldsymbol{b}_C$$
fluxes over cell faces

Theory and Classification



The analytical solution to any differential equation is obtained up to some constants that are fixed by the applicable boundary conditions to the situation being studied.

- Therefore, using different boundary conditions will result in different solutions even though the general equation remains the same.
- Numerical solutions follow the same constraint, necessitating correct and accurate implementation of boundary conditions as any slight change in these conditions introduced by the numerical approximation leads to a wrong solution of the problem under consideration.

The nature of the boundary conditions is strictly related to the terms being discretized. The main types of boundary conditions for conduction/diffusion problems are:

- fixedValue (Dirichlet)
- zeroGradient (Neumann)
- mixed
- symmetry

This classification is the same that can be found in OpenFOAM.

Boundary conditions - Spatial Discretization



Boundary conditions are applied on boundary elements, which have one or more faces on the boundary. Discrete values of ϕ are stored both at centroids of boundary cells and at centroids of boundary faces.

Let's consider the discretization of the diffusion term in the NS equations:

$$-\nabla \cdot (\Gamma \nabla \phi) = -\sum_f \left(\Gamma^\phi \nabla \phi\right)_f \boldsymbol{S}_f = -\sum_f \left(\boldsymbol{J}_f \boldsymbol{S}_f\right)$$

being:

$$\mathbf{J}_f = -\Gamma_f \left(\Delta x\right)_f \left(\frac{\partial \phi}{\partial x}\right)_f$$

If $\left(\frac{\partial \phi}{\partial x}\right)_f$ need to be calculated near the boundary, the boundary condition need to provide the value of ϕ_f .

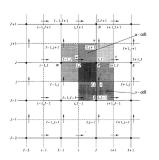
Face-addressing scheme in OpenFOAM



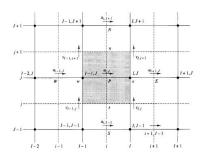
The evaluation of the fluxes at the faces of a **domain boundary** does not require, in general, a profile assumption. **Rather a direct substitution is usually performed.**

Choice of Variable Arrangement on the Grid





Staggered grid arrangement



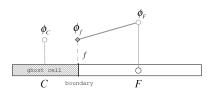
Colocated grid arrangement

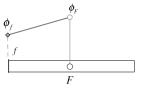
We have already seen that:

- in the staggered arrangement introduced by Harlow and Welsh (1965), both pressure and diffusion terms are very naturally approximated by CD approximations without interpolation; a strong coupling between the velocities and the pressure is achieved.
- the colocated variable arrangement allows significant advantages in complicated solution domains, especially when the boundaries have slope discontinuities or the boundary conditions are discontinuous

Flux Calculation at the Boundary







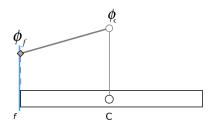
Flux at the boundary: staggered grid (left), collocated arrangement (right).

Depending on the variable arrangement adopted by the CFD code in use, the implementation strategy for the boundary conditions is different. In the following, we will refer to the **colocated variable arrangement**, which is used in OpenFOAM.

In OpenFOAM:

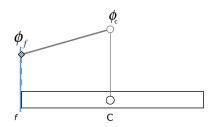
- the ghost cell does not exist and flux is applied directly at the boundary face;
- the class fvPatchField is the base class for all the boundary conditions available in the code for scalar and vector quantities.





It is important to note that at the boundary a the linear profile is assumed for the variation of ϕ between the cell center and the face center. This is a major approximation which is very common in a FV framework and it ensures the boundedness of ϕ .



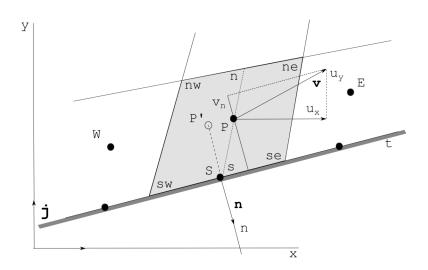


Usually:

- CONVECTIVE FLUXES are prescribed at the inflow boundary. Convective fluxes are zero at impermeable walls and symmetry planes, and are usually assumed to be independent of the coordinate normal to an outflow boundary;
- DIFFUSIVE FLUXES are sometimes specified at a wall e.g. specified heat flux (including the special case of an adiabatic surface with zero heat flux) or boundary values of variables are prescribed.
- If the GRADIENT itself is specified, it is used to calculate the flux, and an approximation for the flux in terms of nodal values can be used to calculate the boundary value of the variable.

Boundary conditions - Spatial Discretization





DIRICHLET Boundary Condition



Dirichlet boundary condition is a type of boundary condition that specifies the value of ϕ at the boundary.

For the element C, the a_{E} coefficient is zero, reducing the equation to:

$$a_C\phi_C + a_W\phi_W + a_N\phi_N + a_S\phi_S = b_C \label{eq:action}$$
 being:

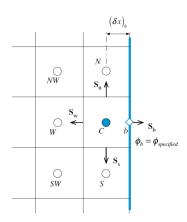
$$a_{E} = 0$$

$$a_{W} = \phi_{w} = -\Gamma_{w} \frac{(\Delta y)_{w}}{\delta x_{w}}$$

$$a_{N} = \phi_{N} = -\Gamma_{n} \frac{(\Delta y)_{n}}{\delta x_{n}}$$

$$a_{S} = \phi_{S} = -\Gamma_{s} \frac{(\Delta y)_{s}}{\delta x_{s}}$$

$$a_{C} = -(a_{E} + a_{W} + a_{N} + a_{S})$$

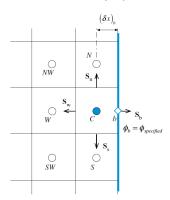


DIRICHLET Boundary Condition



The following important observations can be made about the discretized boundary equation:

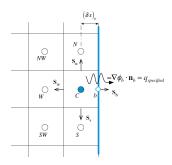
- The coefficient a_b is larger than other neighbor coefficients because b is closer to C and consequently has a more important effect on ϕ_C .
- The coefficient a_C is still the sum of all neighboring coefficients including a_b . This means that for the boundary element $\sum_f |a_F|/|a_C| < 1$ giving the second necessary condition to satisfy the Scarborough criterion, thus guaranteeing, at any one iteration, the convergence of the linear system of equations via an iterative solution method.
- The $a_b\phi_b$ product is now on the right hand side of the equation, i.e., part of b_C , because it does not contain unknowns.



NEUMANN Boundary Condition



If the flux (or normal gradient to the face) of ϕ is specified at the boundary, then the boundary condition is denoted by a Neumann boundary condition.

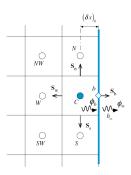


In this case the specified flux is given by

$$-\left(\Gamma\nabla\phi\right)_{b}\boldsymbol{i}=q_{b}$$

MIXED Boundary Condition





The mixed boundary condition refers to the situation where information at the boundary is given via a convection transfer coefficient (h_{∞}) and a surrounding value for $\phi(\phi_{\infty})$ as:

$$-(\Gamma \nabla \phi)_b \, \mathbf{i} \, S_b = -h_\infty (\phi_\infty - \phi_b) (\Delta y)_c$$

IMPORTANT!



IMPORTANT NOTE: boundary conditions **MUST** be set **FOR EACH** equation (e.g. linear system) to solve. So, for each unknown of the equations you are going to solve for (pressure, velocity, internal energy/enthalpy, transported scalar quantity...), you need to specify boundary conditions!

The class fvPatchField<Type> in OF



The main basic boundary condition types available in OpenFOAM are:

- fixedValue: value of ϕ_b is specified by value.
- fixedGradient: normal gradient of $\phi_b\left(\frac{\partial \phi_b}{\partial n}\right)$ is specified by gradient.
- zeroGradient: normal gradient of ϕ_b is zero.
- calculated: patch field ϕ_b calculated from other patch fields.

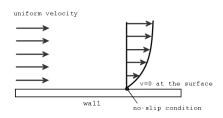
This is not a complete list; for all types, please see:

\$FOAM_SRC/finiteVolume/fields/fvPatchFields/basic.

Examples: NO-SLIP



Example 1: NO-SLIP boundary condition



At a wall the no-slip boundary condition applies, i.e. the velocity of the fluid is equal to the wall velocity (Dirichlet boundary condition). However, there is another condition that can be directly imposed in a FV method; the normal viscous stress is zero at a wall. This follows from the continuity equation, e.g. for a wall at y=0

$$\left(\frac{\partial u}{\partial x}\right)_{\text{wall}} = 0 \Rightarrow \left(\frac{\partial v}{\partial y}\right) = 0 \Rightarrow \tau_{xx} = 2\mu \left(\frac{\partial v}{\partial y}\right) = 0$$

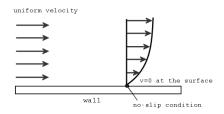
Therefore, the diffusive flux in the v equation at the south boundary is:

$$F_s^d = \int_{S_s} \tau_{yy} dS = 0$$

Examples: NO-SLIP



Example 1: NO-SLIP boundary conditions



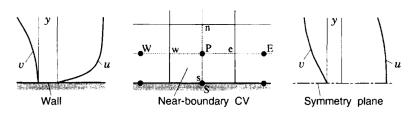
This should be implemented directly, rather than using only the condition that ${\bf v}=0$ at the wall. Since $v_p \neq 0$, we would obtain a non-zero derivative in the discretized flux expression if this were not done; v=0 is used as a boundary condition in the continuity equation. The shear stress can be calculated by using a one-sided approximation of the derivative $\partial u/\partial y$; one possible approximation is:

$$F_s^d = \int_{S_e} \tau_{xy} \, dS = \int_{S_e} \mu \frac{\partial u}{\partial y} dS \simeq \mu_s S_s \frac{u_P - u_S}{y_P - y_S}$$

Examples: symmetry plane



Example 2: SYMMETRY planes b.c.



At a symmetry plane, the shear stress is zero, but the normal stress is not, since:

$$\left(\frac{\partial u}{\partial y}\right)_{\text{sym}} = 0 \qquad \left(\frac{\partial v}{\partial y}\right)_{\text{sym}} \neq 0$$

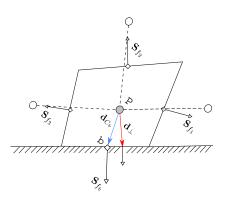
The diffusive flux in the u equation is zero, and the diffusive flux in the v equation can be approximated as:

$$F_s^d = \int_{S_e} \tau_{yy} \, dS = \int_{S_e} 2 \, \mu \frac{\partial v}{\partial y} dS \simeq \mu_s S_s \frac{v_P - v_S}{y_P - y_S}$$

where $v_s = 0$ applies.

Dirichlet b.c.: an example





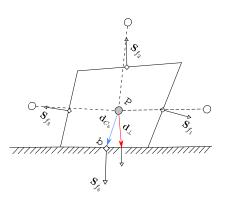
Consider the case where some scalar ϕ is being convected through an inlet. Assuming the diffusion of ϕ to be negligible, the boundary condition can be expressed as:

$$\phi_b = \phi_{b, \text{specified}}$$

For the boundary face, the boundary flux is evaluated using the known value of Φ_b . As a direct consequence, the linear coefficient for the convection term is directly evaluated, since the boundary flux is known, using the midpoint rule.

Dirichlet b.c.: an example





Since the normal velocity is constant along cell faces, we express the convective flux as a product of the mass flux and the mean value of ϕ as:

$$F_e^C = \int_{S_e} \rho \phi \boldsymbol{u} \cdot \boldsymbol{n} dS \simeq \dot{m}_e \phi_e$$

where \dot{m}_e is the mass flux through the 'e' face:

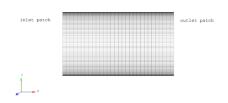
$$\dot{m}_e = \int_{S_e} \rho \boldsymbol{u} \cdot \boldsymbol{n} dS = (\rho u_x)_e \, \Delta y$$

Prescribed Mass Flux Through a Boundary



Prescribed mass flux through a boundary

1. When the mass flux through a boundary is prescribed, the mass flux correction in the pressure correction equation is also zero there; this condition should be directly implemented in the continuity equation when deriving the pressure-correction equation. This is equivalent to specifying a Neumann boundary condition (zero gradient) for the pressure correction.



inlet patch:

- velocity: fixedValue $\rightarrow v = v_{in}$
- pressure: zeroGradient $\rightarrow \frac{\partial p}{\partial x} = 0$

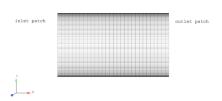
outlet patch:

- velocity: zeroGradient $ightarrow rac{\partial v}{\partial x} = 0$
- pressure: fixedValue ightarrow p = 0

Prescribed Mass Flux Through a Boundary



- 2. At the outlet, if the inlet mass fluxes are given, extrapolation of the velocity to the boundary (zeroGradient, e.g. $U_E=u_p$) can usually be used for steady flows when the outflow boundary is far from the region of interest and the Reynolds number is large.
 - The extrapolated velocity is then corrected to give exactly the same total mass flux as at inlet (this cannot be guaranteed by any extrapolation).
 - The corrected velocities are then considered as prescribed for the following outer iteration and the mass flux correction at the outflow boundary is set to zero in the continuity equation.



inlet patch:

- velocity: fixedValue $\rightarrow v = v_{in}$
- pressure: zeroGradient $\rightarrow \frac{\partial p}{\partial x} = 0$

outlet patch:

- velocity: zeroGradient $\rightarrow \frac{\partial v}{\partial x} = 0$
- pressure: fixedValue $\rightarrow p = 0$

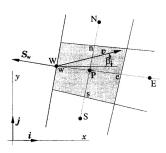
Total quantities



These boundary conditions also hold for compressible flow and are treated in the same way as in incompressible flows. However, in compressible flow there are further boundary conditions:

- prescribed total pressure;
- prescribed total temperature;
- prescribed static pressure on the outflow boundary;
- at a supersonic outflow boundary, zero gradients of all quantities are usually specified.





For isentropic flow of an ideal gas, the total pressure is defined as:

$$p_t = p \left(1 + \frac{\gamma - 1}{2} \frac{u_x^2 + u_y^2}{\gamma RT} \right)^{\frac{\gamma}{\gamma - 1}}$$

where p is the static pressure and $\gamma=c_p/c_v$. The flow direction must be prescribed; it is defined by:

$$\tan \beta = \frac{u_y}{u_x}$$

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These boundary conditions can be implemented by extrapolating the pressure from the interior of the solution domain to the boundary and then calculating the velocity there with the aid of the equation for the conservation of the total pressure.

- These velocities can be treated as known within an outer iteration.
- The temperature can be prescribed or it can be calculated from the total temperature:

$$T_t = T \left(1 + \frac{\gamma - 1}{2} \frac{u_x^2 + u_y^2}{\gamma RT} \right)$$

This treatment leads to slow convergence of the iterative method as there are many combinations of pressure and velocity that satisfy the conservation of total pressure, since the consideration of the influence of the pressure on the velocity at the inflow is implicit. **There is an alternative way of doing this.**



Calculation of the Total Pressure B.C. (1/2)

- At the beginning of an outer iteration the velocities at the inflow boundary must be computed from the equations described abovel they will then be treated as fixed during the outer iteration of the momentum equation.
- The mass fluxes at the inflow are taken from the preceding outer iteration; they should satisfy the continuity equation.
- From the solution of the momentum equation, a new mass flux \dot{m}^* is computed. The 'prescribed' velocities on the inflow boundary are used to compute the mass flux there.
- In the following correction step, the mass flux (including its value at the inflow boundary) is corrected and mass conservation is enforced. The difference between the mass flux correction on the boundary and that at interior control volume faces is that, at the boundary, only the velocity and not the density is corrected. The velocity correction is expressed in terms of the pressure correction and not its gradient:

$$u'_{w} = \left(\frac{\partial u}{\partial p}\right)_{w} p'_{w} = C_{u} p'_{w}$$

where the correction is applied to C_u .



Calculation of the Total Pressure B.C. (2/2)

- The pressure **correction** at the boundary is expressed by means of extrapolation from the center of the neighboring control volume and a contribution to the coefficients A_p and A_E in the pressure correction equation for the control volume next to the boundary is added.
- Since the density is not corrected at the inflow, there is no convective contribution to the pressure correction equation :

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \left[\frac{\partial (\psi \cdot p)}{\partial t} + \nabla \cdot (\rho^* \mathbf{u}^*) \right]$$

- After solution of the pressure correction equation, the velocity components and the mass fluxes in the entire domain including the inflow boundary are corrected. The corrected mass fluxes satisfy the continuity equation within the convergence tolerance. These are used to compute the coefficients in all of the transport equations for the next outer iteration. The convective velocities at the inflow boundary are re-computed. The pressure adjusts itself so that the velocity satisfies the continuity equation and the boundary condition on the total pressure. The temperature at the inflow is calculated and the density from the equation of state.



Thank you for your attention!

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