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Introductory OpenFOAM® Course

From 8th to 12th July, 2013

University of Genoa, DICCA

Dipartimento di Ingegneria Civile, Chimica e Ambientale



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Acknowledgements

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Today's lecture

1. Finite Volume Method: A Crash Introduction

Finite Volume Method: A Crash introduction

**Before continuing,
I want to remind you that this
is not a FVM/CFD course**

Finite Volume Method: A Crash introduction

My favorite FVM/CFD references:

- **An Introduction to Computational Fluid Dynamics.**
H. K. Versteeg, W. Malalasekera. 2007, Prentice Hall.
- **Computational Methods for Fluid Dynamics.**
J. H. Ferziger, M. Peric. 2001, Springer.
- **Computational Fluid Dynamics: Principles and Applications.**
J. Blazek. 2006, Elsevier Science.
- **Numerical Heat Transfer and Fluid Flow.**
S. Patankar. 1980, Taylor & Francis
- **Error analysis and estimation in the Finite Volume method with applications to fluid flows.**
H. Jasak. PhD Thesis, 1996. Imperial College, London.
- **A Finite Volume Method for the Prediction of Three-Dimensional Fluid Flow in Complex Ducts.**
M. Peric. PhD Thesis, 1985. Imperial College, London.

Finite Volume Method: A Crash introduction

- Let us use the general transport equation as the starting point to explain the FVM,

$$\underbrace{\int_{V_P} \frac{\partial \rho \phi}{\partial t} dV}_{\text{temporal derivative}} + \underbrace{\int_{V_P} \nabla \cdot (\rho \mathbf{u} \phi) dV}_{\text{convective term}} - \underbrace{\int_{V_P} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) dV}_{\text{diffusion term}} = \underbrace{\int_{V_P} S_\phi(\phi) dV}_{\text{source term}}$$

- We want to solve the general transport equation for the transported quantity ϕ in a given domain, with given boundary conditions and initial conditions.
- This is a second order equation. For good accuracy, it is necessary that the order of the discretization is equal or higher than the order of the equation that is being discretized.
- Hereafter we are going to assume that the discretization practice is at least second order accurate in space and time.

Finite Volume Method: A Crash introduction

- Let us use the general transport equation as the starting point to explain the FVM,

$$\underbrace{\int_{V_P} \frac{\partial \rho \phi}{\partial t} dV}_{\text{temporal derivative}} + \underbrace{\int_{V_P} \nabla \cdot (\rho \mathbf{u} \phi) dV}_{\text{convective term}} - \underbrace{\int_{V_P} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) dV}_{\text{diffusion term}} = \underbrace{\int_{V_P} S_\phi(\phi) dV}_{\text{source term}}$$

- Hereafter we are going to assume that the discretization practice is at least second order accurate in space and time.
- As consequence of this requirement, all dependent variables are assumed to vary linearly around a point P in space and instant t in time,

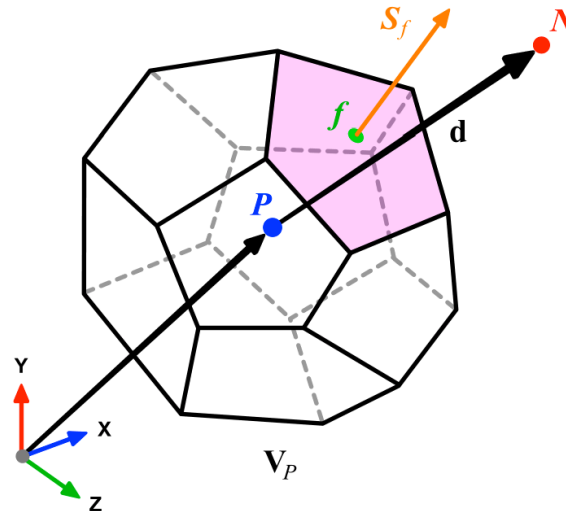
$$\phi(\mathbf{x}) = \phi_P + (\mathbf{x} - \mathbf{x}_P) \cdot (\nabla \phi)_P \quad \text{where} \quad \phi_P = \phi(\mathbf{x}_P)$$

$$\phi(t + \delta t) = \phi^t + \delta t \left(\frac{\partial \phi}{\partial t} \right)^t \quad \text{where} \quad \phi^t = \phi(t)$$

PROFILE ASSUMPTIONS

Finite Volume Method: A Crash introduction

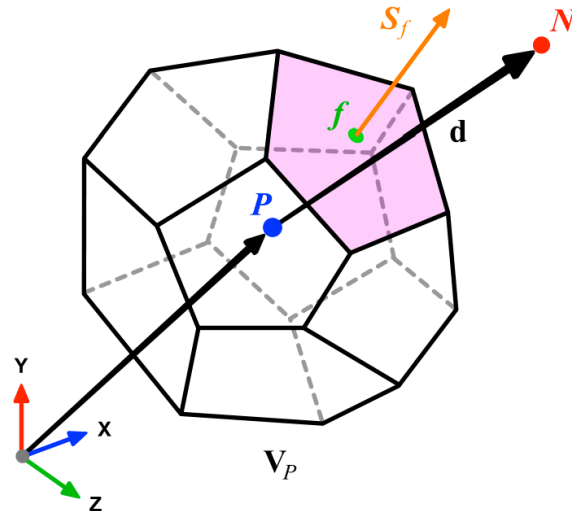
- Let us divide the solution domain into arbitrary control volumes such as the one illustrated below.



- The control volume V_P has a volume V and is constructed around point P , which is the centroid of the control volume. Therefore the notation V_P .
- The vector from centroid P of V_P to centroid N of V_N is named \mathbf{d} .
- The control volume faces are labeled f , which also denotes the face center.
- The face area vector \mathbf{S}_f point outwards from the control volume, is located at the face centroid, is normal to the face and has a magnitude equal to the area of the face.

Finite Volume Method: A Crash introduction

- Let us divide the solution domain into arbitrary control volumes such as the one illustrated below.



- In the control volume illustrated, the centroid is given by

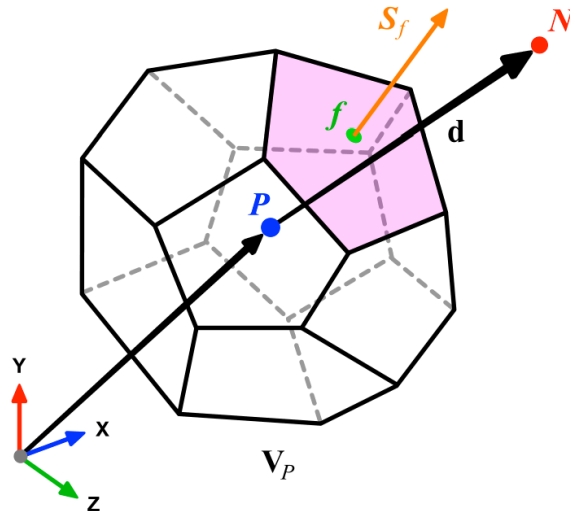
$$\int_{V_P} (\mathbf{x} - \mathbf{x}_P) dV = 0$$

- In the same way, the centroid of face f is given by

$$\int_{S_f} (\mathbf{x} - \mathbf{x}_P) dS = 0$$

Finite Volume Method: A Crash introduction

- Let us divide the solution domain into arbitrary control volumes such as the one illustrated below.



- Finally, we assume that the values of all variables are computed and stored in the centroid of the control volume V_P and that they are represented by a piecewise constant profile,

$$\phi_P = \bar{\phi} = \frac{1}{V_P} \int_{V_P} \phi(\mathbf{x}) dV$$

- This is known as the collocated arrangement.

VARIABLE ARRANGEMENT AND MEAN VALUE ASSUMPTIONS

Finite Volume Method: A Crash introduction

- Let us integrate the general transport equation in space over arbitrary control volumes, this yields to

$$\underbrace{\int_{V_P} \frac{\partial \rho \phi}{\partial t} dV}_{\text{temporal derivative}} + \underbrace{\int_{V_P} \nabla \cdot (\rho \mathbf{u} \phi) dV}_{\text{convective term}} - \underbrace{\int_{V_P} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) dV}_{\text{diffusion term}} = \underbrace{\int_{V_P} S_\phi(\phi) dV}_{\text{source term}}$$

- Next, we recall the Gauss's theorem,

$$\int_V \nabla \cdot \mathbf{a} dV = \oint_{\partial V} d\mathbf{S} \cdot \mathbf{a}$$

where ∂V_P is a closed surface bounding the control volume V_P and $d\mathbf{S}$ represents an infinitesimal surface element with associated normal \mathbf{n} pointing outward of the the surface ∂V_P .

- Notice that

$$\mathbf{n} dS = d\mathbf{S}$$

Finite Volume Method: A Crash introduction

- Let us integrate the general transport equation in space over arbitrary control volumes, this yields to

$$\underbrace{\int_{V_P} \frac{\partial \rho \phi}{\partial t} dV}_{\text{temporal derivative}} + \underbrace{\int_{V_P} \nabla \cdot (\rho \mathbf{u} \phi) dV}_{\text{convective term}} - \underbrace{\int_{V_P} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) dV}_{\text{diffusion term}} = \underbrace{\int_{V_P} S_\phi(\phi) dV}_{\text{source term}}$$

- Hereafter, we use the Gauss's theorem to convert the volume integrals into surface integrals,

- $$\frac{\partial}{\partial t} \int_{V_P} (\rho \phi) dV + \oint_{\partial V_P} \underbrace{d\mathbf{S} \cdot (\rho \mathbf{u} \phi)}_{\text{convective flux}} - \oint_{\partial V_P} \underbrace{d\mathbf{S} \cdot (\rho \Gamma_\phi \nabla \phi)}_{\text{diffusive flux}} = \int_{V_P} S_\phi(\phi) dV$$

Finite Volume Method: A Crash introduction

- Integrating in space each term of the general transport equation and by using Gauss's theorem, yields to the following discrete equations for each term

Convective term:

$$\int_{V_P} \underbrace{\nabla \cdot (\rho \mathbf{u} \phi)}_{\text{convective term}} dV = \oint_{\partial V_P} \underbrace{d\mathbf{S} \cdot (\rho \mathbf{u} \phi)}_{\text{convective flux}} = \sum_f \int_f d\mathbf{S} \cdot (\rho \mathbf{u} \phi)_f \approx \underbrace{\sum_f \mathbf{S}_f \cdot (\overline{\rho \mathbf{u} \phi})_f}_{\text{approximation}} = \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f$$

where we have approximated the integrant by means of the mid point rule, which is second order accurate

Diffusive term:

$$\int_{V_P} \underbrace{\nabla \cdot (\rho \Gamma_\phi \nabla \phi)}_{\text{diffusion term}} dV = \oint_{\partial V_P} \underbrace{d\mathbf{S} \cdot (\rho \Gamma_\phi \nabla \phi)}_{\text{diffusive flux}} = \sum_f \int_f d\mathbf{S} \cdot (\rho \Gamma_\phi \nabla \phi)_f \approx \underbrace{\sum_f \mathbf{S}_f \cdot (\overline{\rho \Gamma_\phi \nabla \phi})_f}_{\text{approximation}} = \sum_f \mathbf{S}_f \cdot (\rho \Gamma_\phi \nabla \phi)_f$$

where we have approximated the integrant by means of the mid point rule, which is second order accurate

Finite Volume Method: A Crash introduction

- Integrating in space each term of the general transport equation and by using Gauss's theorem, yields to the following discrete equations for each term

Source term:

$$\int_{V_P} S_\phi(\phi) dV = S_c V_P + S_p V_P \phi_P$$

This approximation is exact if S_ϕ is either constant or varies linearly within the control volume; otherwise it is second order accurate
 S_c is the constant part of the source term and
 S_p is the non-linear part

Gradient term:

$$(\nabla \phi)_P = \frac{1}{V_P} \sum_f (\mathbf{S}_f \phi_f)$$

where we have approximated the centroid gradients by using the Gauss theorem.
This method is second order accurate

Finite Volume Method: A Crash introduction

- Integrating in space each term of the general transport equation and by using Gauss's theorem, yields to the following discrete equations for each term

Convective term:

$$\int_{V_P} \underbrace{\nabla \cdot (\rho \mathbf{u} \phi)}_{\text{convective term}} dV = \oint_{\partial V_P} \underbrace{d\mathbf{S} \cdot (\rho \mathbf{u} \phi)}_{\text{convective flux}} = \sum_f \int_f d\mathbf{S} \cdot (\rho \mathbf{u} \phi)_f \approx \sum_f \mathbf{S}_f \cdot (\overline{\rho \mathbf{u} \phi})_f = \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f$$

Diffusive term:

$$\int_{V_P} \underbrace{\nabla \cdot (\rho \Gamma_\phi \nabla \phi)}_{\text{diffusion term}} dV = \oint_{\partial V_P} \underbrace{d\mathbf{S} \cdot (\rho \Gamma_\phi \nabla \phi)}_{\text{diffusive flux}} = \sum_f \int_f d\mathbf{S} \cdot (\rho \Gamma_\phi \nabla \phi)_f \approx \sum_f \mathbf{S}_f \cdot (\overline{\rho \Gamma_\phi \nabla \phi})_f = \sum_f \mathbf{S}_f \cdot (\rho \Gamma_\phi \nabla \phi)_f$$

Source term:

$$\int_{V_P} S_\phi(\phi) dV = S_c V_P + S_p V_P \phi_P$$

Gradient term:

$$(\nabla \phi)_P = \frac{1}{V_P} \sum_f (\mathbf{S}_f \phi_f)$$

Finite Volume Method: A Crash introduction

- Using the previous equations to evaluate the general transport equation over all the control volumes, we obtain the following semi-discrete equation

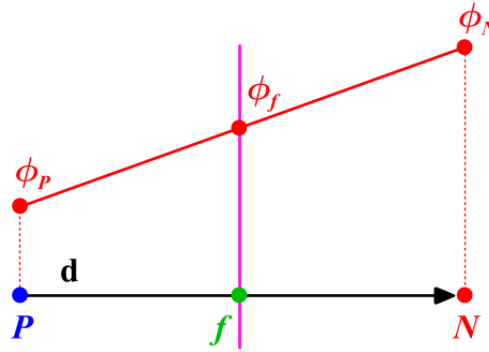
$$\underbrace{\int_{V_P} \frac{\partial \rho \phi}{\partial t} dV}_{\text{temporal derivative}} + \sum_f \underbrace{\mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f}_{\text{convective flux}} - \sum_f \underbrace{\mathbf{S}_f \cdot (\rho \Gamma_\phi \nabla \phi)_f}_{\text{diffusive flux}} = \underbrace{(S_c V_P + S_p V_P \phi_P)}_{\text{source term}}$$

where $F^C = \mathbf{S} \cdot (\rho \mathbf{u} \phi)$ is the convective flux and $F^D = \mathbf{S} \cdot (\rho \Gamma_\phi \nabla \phi)$ is the diffusive flux.

- Recalling that all variables are computed and stored at the centroid of the control volumes. The face values appearing in the convective and diffusive fluxes have to be computed by some form of interpolation from the centroid values of the control volumes at both sides of face f .

Finite Volume Method: A Crash introduction

- By looking the figure below, the face values appearing in the convective flux can be computed as follows,



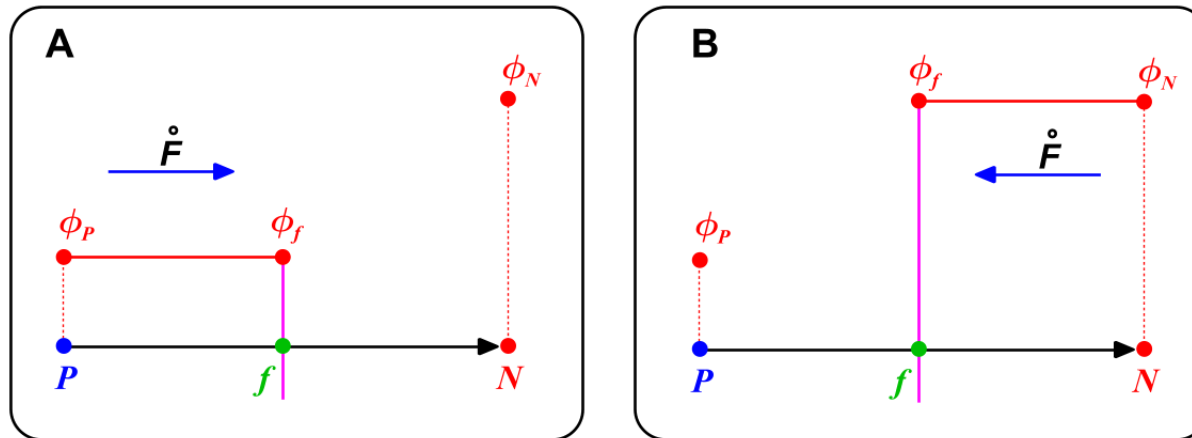
$$\phi_f = f_x \phi_P + (1 - f_x) \phi_N$$

$$f_x = \frac{fN}{PN} = \frac{|\mathbf{x}_f - \mathbf{x}_N|}{|\mathbf{d}|}$$

- This type of interpolation scheme is known as linear interpolation or central differencing and it is second order accurate. However, it may generate oscillatory solutions (unbounded solutions).

Finite Volume Method: A Crash introduction

- By looking the figure below, the face values appearing in the convective flux can be computed as follows,

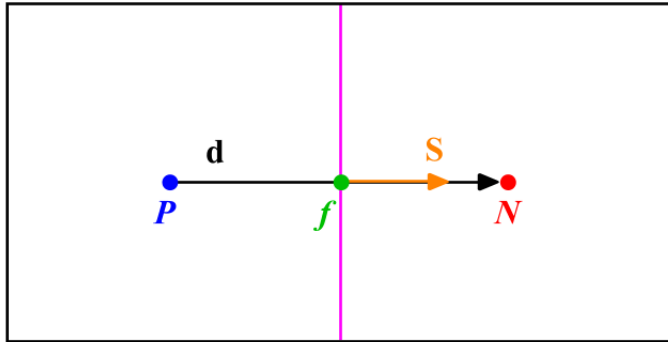


$$\phi_f = \begin{cases} \phi_f = \phi_P & \text{for } \dot{F} \geq 0, \\ \phi_f = \phi_N & \text{for } \dot{F} < 0. \end{cases}$$

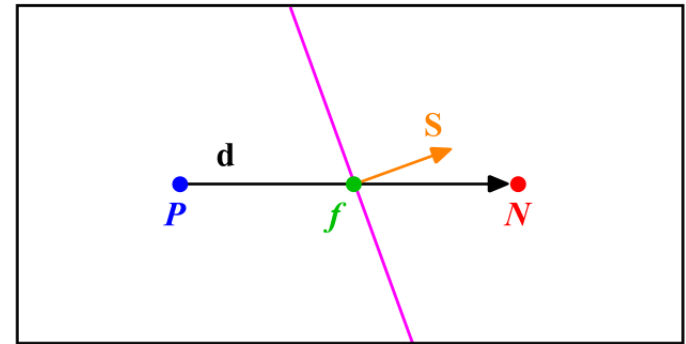
- This type of interpolation scheme is known as upwind differencing and it is first order accurate. This scheme is bounded.

Finite Volume Method: A Crash introduction

- By looking the figures below, the face values appearing in the diffusive flux in an orthogonal mesh can be computed as follows,



Orthogonal mesh

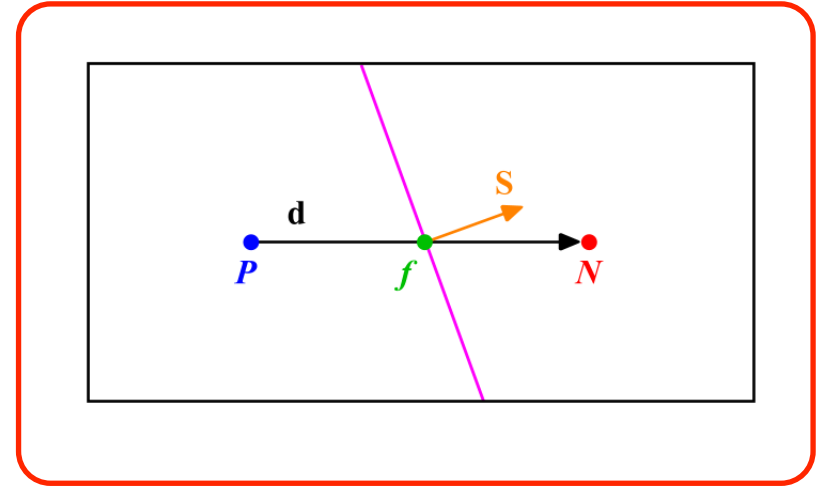
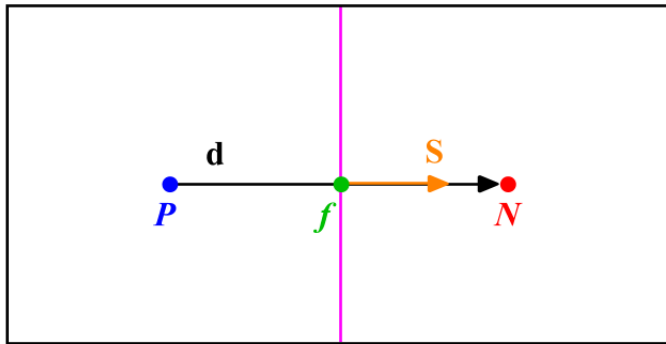


$$\mathbf{S} \cdot (\nabla \phi)_f = |\mathbf{S}| \frac{\phi_N - \phi_P}{|\mathbf{d}|}.$$

- This is a central difference approximation of the first order derivative. This type of approximation is second order accurate.

Finite Volume Method: A Crash introduction

- By looking the figures below, the face values appearing in the diffusive flux in a non-orthogonal mesh can be computed as follows,



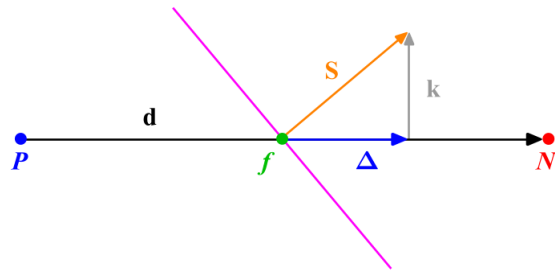
Non-orthogonal mesh

$$\mathbf{S} \cdot (\nabla \phi)_f = \underbrace{|\Delta_{\perp}| \frac{\phi_N - \phi_P}{|d|}}_{\text{orthogonal contribution}} + \underbrace{\mathbf{k} \cdot (\nabla \phi)_f}_{\text{non-orthogonal contribution}}.$$

- This type of approximation is second order accurate but involves a larger truncation error. It also uses a larger numerical stencil, which make it less stable.

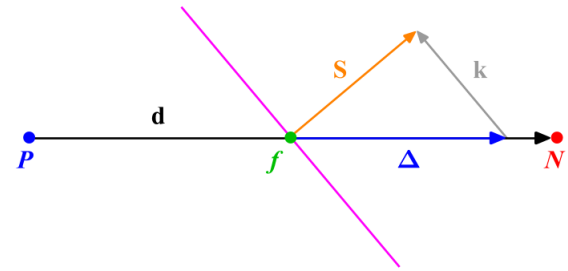
Finite Volume Method: A Crash introduction

- By looking the figures below, the face values appearing in the diffusive flux in a non-orthogonal mesh can be computed as follows,



Minimum correction approach

$$\Delta_{\perp} = \frac{\mathbf{d} \cdot \mathbf{S}}{\mathbf{d} \cdot \mathbf{d}} \mathbf{d}.$$



Over-relaxed approach

$$\Delta_{\perp} = \frac{\mathbf{d}}{\mathbf{d} \cdot \mathbf{S}} |\mathbf{S}|^2.$$

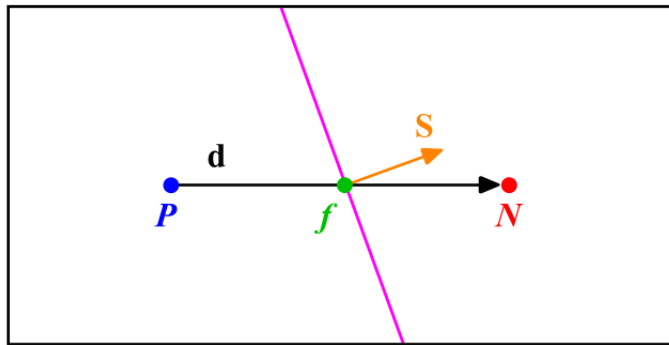
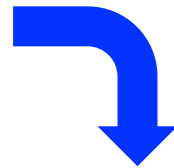
$$\mathbf{S} = \Delta_{\perp} + \mathbf{k}.$$

$$\mathbf{S} \cdot (\nabla \phi)_f = \underbrace{|\Delta_{\perp}| \frac{\phi_N - \phi_P}{|\mathbf{d}|}}_{\text{orthogonal contribution}} + \underbrace{\mathbf{k} \cdot (\nabla \phi)_f}_{\text{non-orthogonal contribution}}.$$

Finite Volume Method: A Crash introduction

- The gradient of the non-orthogonal contribution is computed by using Gauss theorem to find the gradient of the control volumes centroid, then the face gradient is found by using linear interpolation.

$$\mathbf{S} \cdot (\nabla \phi)_f = \underbrace{|\Delta_{\perp}| \frac{\phi_N - \phi_P}{|\mathbf{d}|}}_{\text{orthogonal contribution}} + \underbrace{\mathbf{k} \cdot (\nabla \phi)_f}_{\text{non-orthogonal contribution}}$$

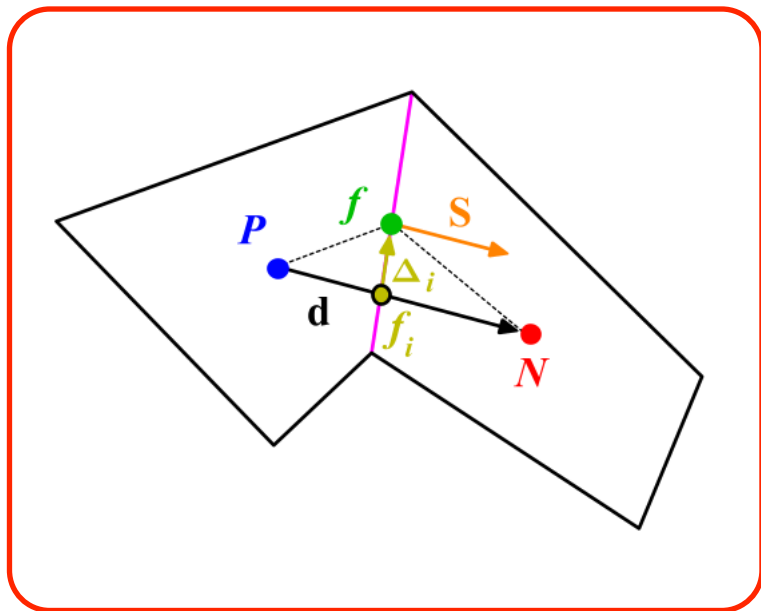


$$\begin{aligned} \int_{V_P} \nabla \phi dV &= \oint_{\partial V_P} d\mathbf{S} \phi \\ (\nabla \phi)_P V_P &= \sum_f (\mathbf{S}_f \phi_f) \\ (\nabla \phi)_P &= \frac{1}{V_P} \sum_f (\mathbf{S}_f \phi_f) \end{aligned}$$

$$(\nabla \phi)_f = f_x (\nabla \phi)_P + (1 - f_x) (\nabla \phi)_N \quad \text{where} \quad f_x = \frac{fN}{PN} = \frac{|\mathbf{x}_f - \mathbf{x}_N|}{|\mathbf{d}|}$$

Finite Volume Method: A Crash introduction

- In the case of a skew mesh (as the one in the figure), we should introduce a correction in order to maintain second order accuracy and avoid unboundedness,



$$1. \quad \phi_f = \phi_{f_i} + \Delta_i \cdot (\nabla \phi)_{f_i}$$

$$2. \quad \phi_{f_i} = f_x \phi_P + (1 - f_x) \phi_N$$

$$\nabla \phi_{f_i} = f_x \nabla \phi_P + (1 - f_x) \nabla \phi_N$$

$$f_x = \frac{f_i N}{P N} = \frac{|\mathbf{x}_{f_i} - \mathbf{x}_N|}{|\mathbf{d}|}.$$

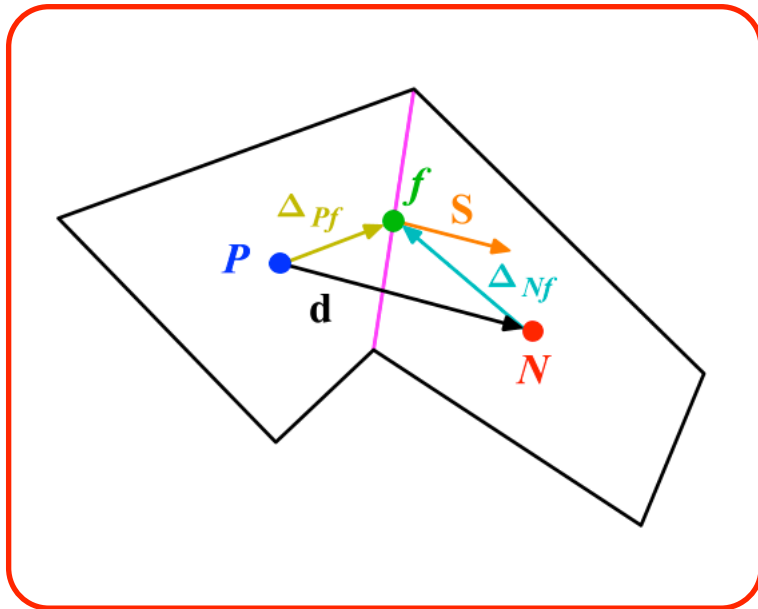
$$3. \quad (\nabla \phi)_P = \frac{1}{V_P} \sum_f \mathbf{S}_f \phi_f = \frac{1}{V_P} \sum_f \mathbf{S}_f \left[\phi_{f_i} + \Delta_i \cdot (\nabla \phi)_{f_i} \right]$$

$$\nabla \phi_{f_i} = \frac{(\phi_N - \phi_P)}{|\mathbf{d}|}$$

Initial approximation of the face gradient

Finite Volume Method: A Crash introduction

- In the case of a skew mesh (as the one in the figure), we should introduce a correction in order to maintain second order accuracy and avoid unboundedness,



$$1. (\nabla\phi)_P = \frac{1}{V_P} \sum_f (\mathbf{S}_f \phi_f)$$

$$2. \phi_f = \frac{(\phi_P + \Delta_{Pf} \cdot \nabla\phi_P) + (\phi_N + \Delta_{Nf} \cdot \nabla\phi_N)}{2}$$

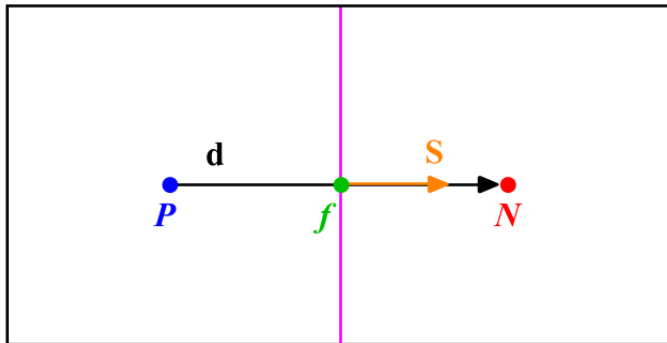
$$3. (\nabla\phi)_f = f_x (\nabla\phi)_P + (1 - f_x) (\nabla\phi)_N$$

$$f_x = \frac{fN}{PN} = \frac{|\mathbf{x}_f - \mathbf{x}_N|}{|\mathbf{d}|}$$

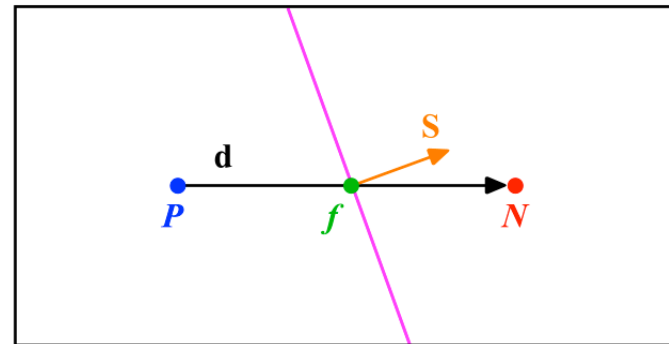
$$\phi_f = \frac{(\phi_P + \phi_N)}{2} \quad \text{and} \quad \nabla\phi_f = \frac{(\nabla\phi_P + \nabla\phi_N)}{2} \quad \text{are the initial approximations}$$

Finite Volume Method: A Crash introduction

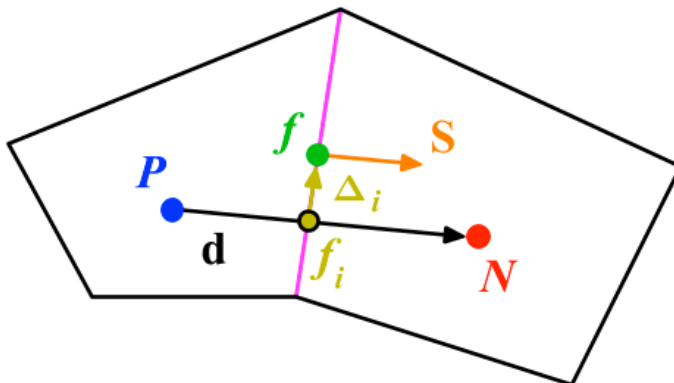
- **Mesh induced errors.** In order to, maintain second order accuracy and to avoid unboundedness, we need to correct non-orthogonality and skewness errors.



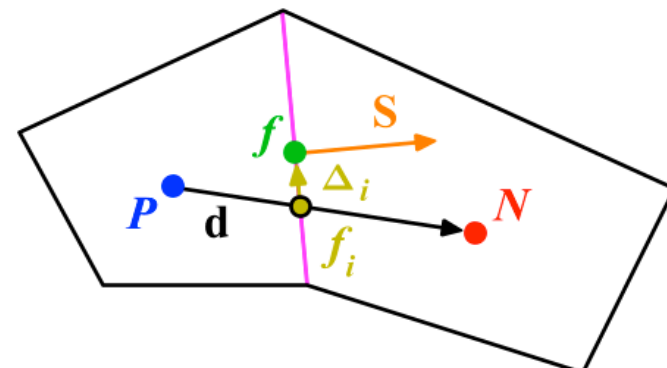
Orthogonal and non skew mesh



Non-orthogonal and non skew mesh



Orthogonal and skew mesh



Non-orthogonal and skew mesh

Finite Volume Method: A Crash introduction

- Using the previous equations to evaluate the general transport equation over all the control volumes, we obtain the following semi-discrete equation

$$\underbrace{\int_{V_P} \frac{\partial \rho \phi}{\partial t} dV}_{\text{temporal derivative}} + \sum_f \underbrace{\mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f}_{\text{convective flux}} - \sum_f \underbrace{\mathbf{S}_f \cdot (\rho \Gamma_\phi \nabla \phi)_f}_{\text{diffusive flux}} = \underbrace{(S_c V_P + S_p V_P \phi_P)}_{\text{source term}}$$

where $F^C = \mathbf{S} \cdot (\rho \mathbf{u} \phi)$ is the convective flux and $F^D = \mathbf{S} \cdot (\rho \Gamma_\phi \nabla \phi)$ is the diffusive flux.

- After spatial discretization, we can proceed with the temporal discretization. By proceeding in this way we are using the Method of Lines (MOL).
- The main advantage of the MOL method, is that it allows us to select numerical approximations of different accuracy for the spatial and temporal terms. Each term can be treated differently to yield to different accuracies.

Finite Volume Method: A Crash introduction

- Now, we evaluate in time the semi-discrete general transport equation

$$\int_t^{t+\Delta t} \left[\left(\frac{\partial \rho \phi}{\partial t} \right)_P V_P + \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f - \sum_f \mathbf{S}_f \cdot (\rho \Gamma_\phi \nabla \phi)_f \right] dt \\ = \int_t^{t+\Delta t} (S_c V_P + S_p V_P \phi_P) dt.$$

- At this stage, we can use any time discretization scheme, *e.g.*, Crank-Nicolson, euler implicit, forward euler, backward differencing, adams-bashforth.
- It should be noted that the order of the temporal discretization of the transient term does not need to be the same as the order of the discretization of the spatial terms. Each term can be treated differently to yield different accuracies. As long as the individual terms are at least second order accurate, the overall accuracy will also be second order.

Finite Volume Method: A Crash introduction

- After spatial and temporal discretization and by using equation

$$\int_t^{t+\Delta t} \left[\left(\frac{\partial \rho \phi}{\partial t} \right)_P V_P + \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f - \sum_f \mathbf{S}_f \cdot (\rho \Gamma_\phi \nabla \phi)_f \right] dt$$

$$= \int_t^{t+\Delta t} (S_c V_P + S_p V_P \phi_P) dt.$$

in every control volume V_P of the domain, a system of linear algebraic equations for the transported quantity ϕ is assembled

$$\begin{pmatrix} a_{11} & a_{12} & & \ddots & & & \\ a_{21} & a_{22} & a_{23} & & \ddots & & \\ & \ddots & \ddots & \ddots & & \ddots & \\ \ddots & & \ddots & \ddots & \ddots & \ddots & \\ & a_S & & a_W & a_P & a_E & a_N \\ & & \ddots & & \ddots & \ddots & \ddots \\ & & & \ddots & & \ddots & \ddots \\ & & & & \ddots & & \ddots \\ & & & & & \ddots & a_{PP} \end{pmatrix} \times \begin{pmatrix} \phi_S \\ \phi_W \\ \phi_P \\ \phi_E \\ \phi_N \end{pmatrix} = \begin{pmatrix} b_S \\ b_W \\ b_P \\ b_E \\ b_N \end{pmatrix}$$

and which can be solved by using any iterative or direct method.

Finite Volume Method: A Crash introduction

So, what does OpenFOAM® do?

It simply discretize in space and time the governing equations in arbitrary polyhedral control volumes over the whole domain. Assembling in this way a large set of linear discrete algebraic equations (DAE), and then it solves this system of DAE to find the solution of the transported quantities.

Therefore, we need to give to OpenFOAM® the following information:

- Discretization of the solution domain or the mesh. This information is contained in the directory **constant/polyMesh**.
- Boundary conditions and initials conditions. This information is contained in the directory **0/**.
- Physical properties such as density, gravity, diffusion coefficient, viscosity, etc. This information is contained in the directory **constant/**.
- Physics involve, such as turbulence modeling, mass transfer, etc. This information is contained in the directories **constant/** and/or **system/**

Finite Volume Method: A Crash introduction

So, what does OpenFOAM® do?

Therefore, we need to give to OpenFOAM® the following information:

- How to discretize in space each term of the governing equations (diffusive, convective, gradient and source terms). This information is set in the **system/fvSchemes** dictionary.
- How to discretize in time the obtained semi-discrete governing equations. This information is set in the **system/fvSchemes** dictionary.
- How to solve the linear system of discrete algebraic equations. This information is set in the **system/fvSolution** dictionary.
- Set runtime parameters and general instructions on how to run the case (such as time step and maximum CFL number). This information is set in the **system/controlDict** dictionary.
- Additionally, we may set sampling and functionObjects for post-processing. This information is contained in the specific dictionaries contained in the directory **system/**.

Thank you for your attention

