ENHANCING IMPLICIT HIGH-ORDER SPECTRAL FINITE VOLUME SCHEMES APPLICABILITY ON UNSTRUCTURED MESHES

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Abstract. *The storage and access of grid files by data structures and topological operators is one the most important goals of geometric modeling research field, which allows an efficient and stable implementation of adaptive refinement mechanisms, cells alignment and access to incidence and adjacency properties from grid elements, representing great concern in the majority of applications from fluid mechanics. In the case of non-structured grids, the cellular decomposition if non-uniform and is better suited by a more sophisticated strategy - topological data struct. This paper shows how a data structure can be extended in order to deal with non-supported types of elements, allowing perform simulations using the spectral finite volume method up to the fourth precision order. The fourth order spectral finite volume method obtains higher spatial resolution, where the control volumes are partitioned into smaller volumes of different types, from triangles to hexagons. In order to use the topological data struct, an extension of the structure was developed in order to hold the new generated grid by the partitioning specified by the spectral finite volume method. The extension represents all partitioned elements locally for each original control volume. Therefore, we performed experiments to validate the usage of the data structure along with existing approaches.*

Keywords: *Spectral Finite Volume, Unstructured Meshes, Numerical Simulation, Topological Data Structure.*

1. INTRODUCTION

This paper scope is in the research area of development of high-order methods suitable for steady and unsteady, subsonic, transonic and supersonic flow problems, i.e., external high-speed aerodynamics. Since in literature some flux vector splitting schemes such as the van Leer and Liou AUSM schemes implemented along with Roe's flux difference splitting scheme presented results with an order of accuracy smaller than the expected in the solutions for unstructured grids, it motivated the study of essentially non-oscillatory (ENO) and weighted essentially non-oscillatory (WENO) schemes.

But, as the reconstruction model used in these schemes relies on gathering neighboring cells for polynomial reconstructions for each cell, both were found to be very demanding on computational resources for resolution orders greater than 3 in 2D or anything greater than second order in 3D. This fact motivated the consideration of the Spectral Finite Volume (SFV) method.

The spectral finite volume was first presented in the work of (Wang, 2002), along with its application for scalar hyperbolic conservation laws of one dimension. The extension of the SFV method for bi-dimensional scalar equations and a study of different limit strategies to capture discontinuities in the solution, was presented by (Wang and Liu, 2002). The same authors also presented the extension for the SFV method for one dimensional conservation law systems, along with a optimization study of the partitions performed by the method (Wang and Liu, 2004).

The first formulation of the SFV method for the Navier-Stokes was developed and presented by (Sun *et al.*, 2006). The usage of the SFV method for diffusive problems was proposed by (Kannan and Wang, 2009), which investigated different formulations for the discretizations of the diffusive terms in SFV method. A comparative study between the SFV and DG (Discontinuous Galerkin Method) methods was made by (Sun and Wang, 2004) and also by (Zhang and Shu, 2005).

The work of (Breviglieri, 2010) applied the SFV scheme in a context of finite volume centered in the cell using non-structured meshes. The Euler equations were used to represent the fluid flow and a spatial discretization scheme of second, third and fourth order of resolution were proposed. Concerning time integration, implicit and explicit were used, and for high resolution were used flux limiters.

This paper presents how to extend a current data structure that do not have support to index all element types needed in the spectral volume method, by using a mapping method used to rebuild each control volume partitioned by the SFV method. Particularly, we show how to extend the structure to index such elements (from triangles to hexagons) up to the fourth order of precision in the SFV method.

The outline of the paper is as follows: Section 2. shows the theoretical formulation of the governing equations used; Section 3. discuss the spectral finite volume method; Section 4. explains how an existing data structure can be modified to index the new elements from the SFV method mesh partitioning; Section 5. shows the performed experiments and results; Finally, section 6. draws conclusions and presents future works.

2. THEORETICAL FORMULATION

We are considering simulations with high numbers of Reynolds, where the molecular transport effects can be ignored. For that, the Euler equations represent the flows discussed, and the viscous terms and heat conduction can be discarded. For the following formulation, we consider only bi-dimensional problems.

The Euler equations in two dimension, written in conservative form can be written as

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} + \frac{\partial \mathbf{F}}{\partial y} = 0, \tag{1}$$

where

$$\mathbf{Q} = \left\{ \begin{array}{c} \rho \\ \rho u \\ \rho v \end{array} \right\}, \mathbf{E} = \left\{ \begin{array}{c} \rho u \\ \rho u^2 + p \\ \rho v u \\ (e+p)\, u \end{array} \right\}, \quad \mathbf{F} \left\{ \begin{array}{c} \rho v \\ \rho u v \\ \rho v^2 + p \\ (e+p)\, v \end{array} \right\} \tag{2}$$

The equation system complete with the expression for the pressure evaluation p for a perfect gas.

$$p = (\gamma - 1) \left[e - \frac{1}{2} \rho \left| \mathbf{u} \right|^2 \right]. \tag{3}$$

In this paper, we solved the two-dimensional Euler equations in integral form as:

$$\frac{\partial}{\partial t} \int_V \mathbf{Q} dV + \int_V (\nabla \cdot \mathbf{P})\, dV = 0 \tag{4}$$

where $\mathbf{P} = \mathbf{E}_{\hat{i}} + \mathbf{F}_{\hat{j}}$. By applying the Gauss theorem in previous equation, it results:

$$\frac{\partial}{\partial t} \int_V \mathbf{Q} dV + \int_S (\mathbf{P} \cdot \mathbf{n})\, dS = 0, \tag{5}$$

where V represents the cell volume, S represents the cell surface and $\mathbf{n}$ is the unitary vector normal to the surface S.

The finite volume method is used in the numerical discretization of the equations, then the Eq. (5), discretized in the finite volume context, face centered, can be rewritten to a control volume i as

$$\frac{\partial \mathbf{Q}_i}{\partial t} = -\frac{1}{V_i} \int_{S_i} (\mathbf{P} \cdot \mathbf{n})\, dS, \tag{6}$$

where $\mathbf{Q_i}$ is the mean value of $\mathbf{Q}$ in time t, in volume control V_i, given by

$$\mathbf{Q_i} = \frac{1}{V_i} \int_{V_i} \mathbf{Q} dV. \tag{7}$$

Therefore, the final formulation to a Euler equations discretization in a two-dimensional finite volume context can be written as:

$$\frac{\partial \mathbf{Q_i}}{\partial t} = -\frac{1}{V_i} \sum_{k=1}^{nf} (\mathbf{E_k} \hat{i} + \mathbf{F_k} \hat{j}) \cdot \mathbf{S_k}, \quad \frac{\partial \mathbf{Q_i}}{\partial t} = \mathbf{R}_i \tag{8}$$

where nf is the number of faces which form the control volume i, s_k is the length of the cell neighbor edge and $\mathbf{R}_i$ is the corresponding residual vector, which is related to the evolution of the time solution variables.

3. ABOUT THE SPECTRAL FINITE VOLUME METHOD

3.1 General Formulation

Integrating the hyperbolic conservation law of the Euler equation written in its integral formulation, for each control volume in each cell and applying the Gauss theorem, results in

$$\frac{d\mathbf{Q}_{i,j}}{dt} = \frac{1}{V_{i,j}} \int_{\partial S_{i,j}} \mathbf{P} \cdot \mathbf{n}\, dS \tag{9}$$

where $V_{i,j}$ is the control volume area and the average of conserved variable are defined by

$$\bar{Q}_{i,j} = \frac{1}{V_{i,j}} \int_{V_{i,j}} \mathbf{Q}\, dV \tag{10}$$

The main difference between this method and the finite volume method is that the conserved variables, obtained by the mean of the control volumes of each spectral volume, in each cell i allow to build a polynomial of degree p that approximate the solution in the cell. The space of approximation of the solution of the SFV method is then the space of parts of continuous polynomials of degree p, which allows an accuracy order of $p+1$.

The polynomial solution in each cell allows to solve the surface integrals on internal edges that compose the CVs with accuracy order $P+1$, using proper gaussian quadratures. As for external edges, which are positioned to divide the SVs, two approximated values for the conserved variables are available by the corresponding polynomial solutions of the two neighbor cells. The contribution of these edges at neighborhood of CVs must be equal in magnitude and opposite in sign. In order to guarantee this, approximated Riemann solvers are used. Therefore, the final expression of the spatial discretization is

$$\begin{aligned}\frac{d\mathbf{Q}_{i,j}}{dt} &= -\frac{1}{V_{i,j}} \sum_{k=1}^{nf} \int_{\partial V_{i,j}} \mathbf{P} \cdot \mathbf{n}\, dS \\ &-\frac{1}{V_{i,j}} \sum_{k=1}^{nf} \int_{\partial V_{i,j}} \mathbf{f} \cdot \mathbf{n}\, dS = \mathbf{R}_{i,j}\end{aligned} \tag{11}$$

where the edges and the area integrals must be calculated by using gaussian quadratures which ensure the desired accuracy order. Given the values of the mean of conserved variables, the residue $\mathbf{R}_{i,j}$ of Eq. (11) can be evaluated following the same procedure used in finite volume method. Note that for $p = 0$, the SFV method becomes the classic method of first order of finite volume.

3.2 Spatial Discretization

For the numerical integration on the flux, consider the Eq. (6), rewritten as

$$\frac{\partial Q_i}{\partial t} = \int_{S_i} (\mathbf{P} \cdot \mathbf{n}) dS = \sum_{r=1}^{nf} \int_{S_r} (\mathbf{f} \cdot \mathbf{n}) dS \tag{12}$$

Due to the fact that $\mathbf{n}$ is constant for each line segment, the right side integration of the Eq. (12) can be done numerically with a quadrature gaussian formula of order k

$$\int_S (\mathbf{P} \cdot \mathbf{n}) dS = \sum_{r=1}^{nf} \sum_{q=1}^{nq} w_{rq} \mathbf{f}(\mathbf{Q}(x_{rq}, y_{rq})) \cdot \mathbf{n}_r S_r + O(S_r h^k) \tag{13}$$

where (x_{rq}, y_{rq}) and w_{rq} are the coordinates of the quadrature gaussian points and the weights in the edge number r of the cell i, respectively. The number of necessary quadrature points in the edge number r is given by $nq = (k+1)/2$, rounded to an integer value.

For the second order scheme, one gaussian quadrature point is used in the integration. Given the points coordinates from an edge, z_1 and z_2, one can obtain the quadrature point as the middle point in the edge $G_1 = 0.5(z_1 + z_2)$. For the schemes of order three and four, two quadrature points are needed in each line segment, and their values are

$$\mathbf{G_1} = \frac{\sqrt{3}+1}{2\sqrt{3}} \mathbf{z_1} + \left(1 - \frac{\sqrt{3}+1}{2\sqrt{3}}\right) \mathbf{z_2} \quad e \quad \mathbf{G_2} = \frac{\sqrt{3}+1}{2\sqrt{3}} \mathbf{z_2} + \left(1 - \frac{\sqrt{3}+1}{2\sqrt{3}}\right) \mathbf{z_1}, \tag{14}$$

Therefore, the calculation of the values for $\mathbf{Q}_i$ in time t for each cell can be evaluated by using the above equations.

4. DATA SCRUCT MAPPING

In this section we describe how we can map partitioned elements of the SFV method inside a topological data structure. We used the Mate Face data structure, though this approach can also be applied on other data structures that index elements in a explicit way. Moreover, we present how to map elements when a fourth order SFV method is applied, resulting a better partitioned mesh and providing best results of the method.

The SFV divides the mesh into control volumes. The formed elements in the mesh can be quadrilaterals, pentagons and even hexagons, turning the mesh hybrid, i.e., composed by different geometric elements (cells).

All created control volumes are hold and accessed from original cells on Mate Face (the spectral volumes). The identification for each control volume is unique, in order to allow the global identification to retrieve properties such as the area and the centroid. So, it is necessary to maintain the association between spectral volumes and its control volumes. For this, it is allocated a corresponding vector between cells, as can be seen in Fig. 1. From the figure, we can note that the relationship between original cells (the spectral volumes) and its control volumes (created by SFV method) are hold in the structure. This association is important for the future evaluation of residues, by reconstruction the element in SFV method.

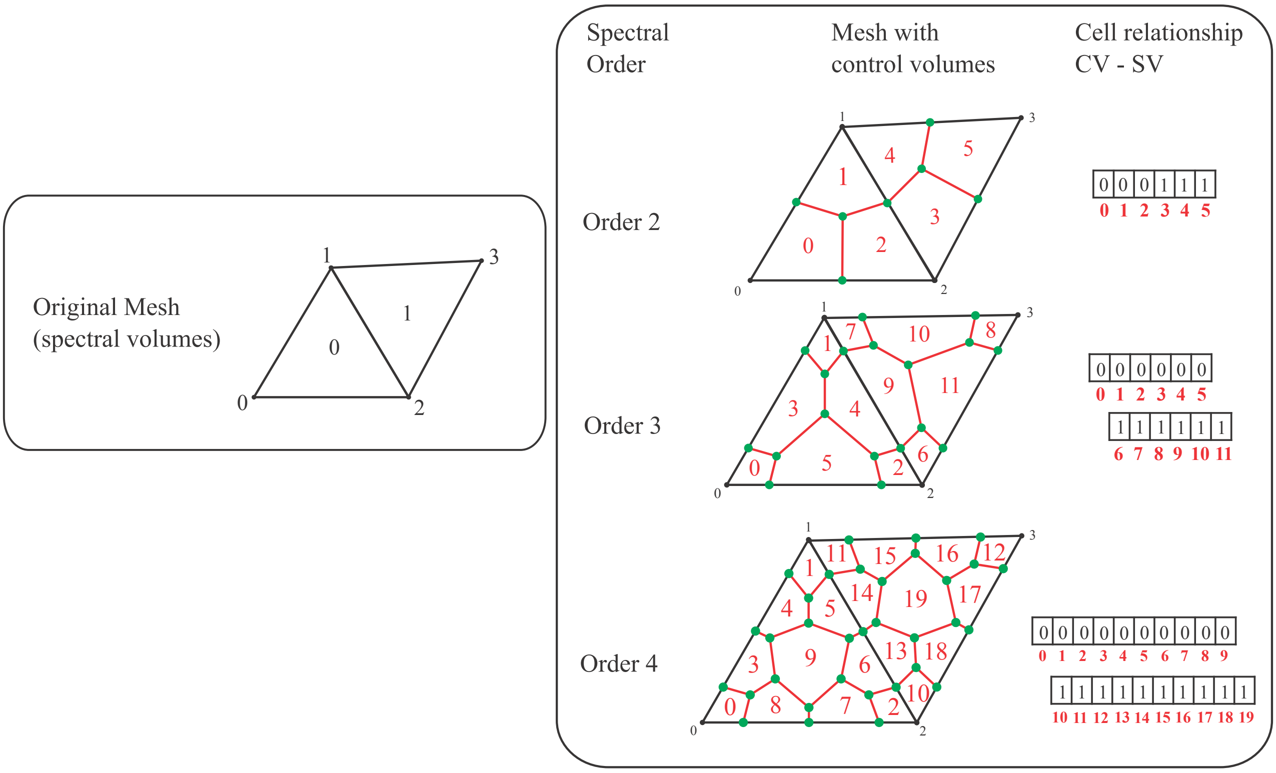


Figure 1. Association between spectral and control volumes for partitioning of second to fourth order of precision.

The labeling of vertexes and cells was made in a way that there is no repetition of labels in a same set of description. Moreover, it must be intuitive to determine which vertex or cell inside a SV cell based only on its label. The label generation is related to the proximity of the original vertex. In this way, the Fig. 2 shows the labeling used in the vertexes and cells resulted from the partitioning of the original cell (spectral volume), according with the spectral order chosen by the user. The labels are mapped to a identification schema of positioning in internal vectors to provide access to the elements information.

Therefore, the formation of control volumes can be made in the data structure as shown in the Fig. 3. The figure shows the internal organization of the spectral volumes according the specified spectral order. Once the labels are semantically associated to its position, formation of internal elements is eased in the matrix of cells of each spectral volume in the mesh, once all of them will present the same partitioning, according to the chosen spectral order.

5. RESULTS

In this section we present experiments to validate our implementation of the mesh partitioning using the data structure Mate Face adapted to index SFV elements by comparing with a non-indexed implementation that uses several matrices pre-computed to describe the mesh. The experiments were performed in a computer Intel I5-3330 3.00GHz with 8Gb RAM under linux Ubuntu operational system.

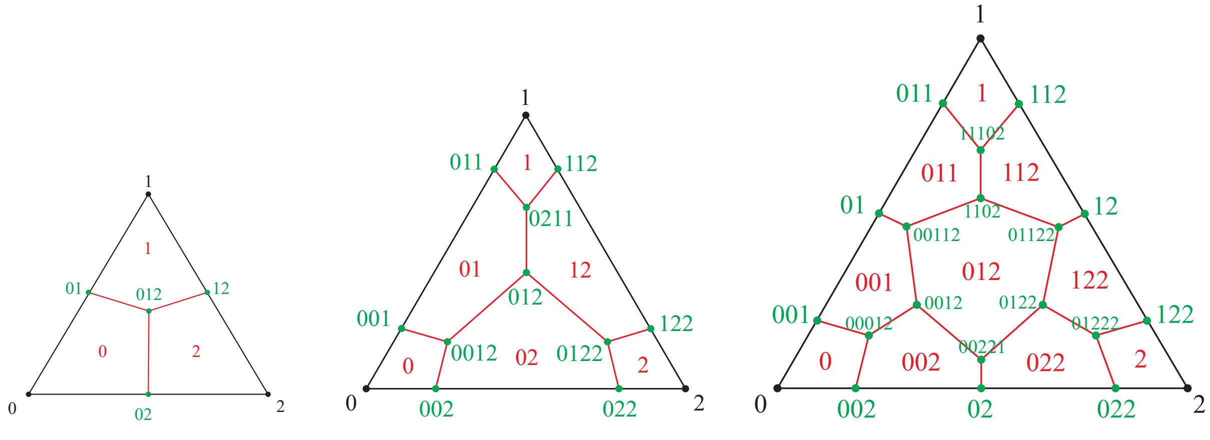
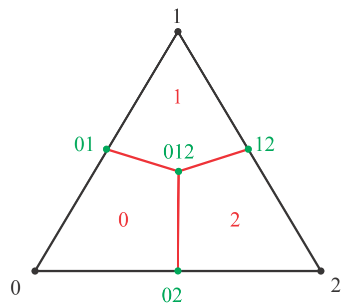


Figure 2. Labeling on control volumes for internal identification.

Spectral Order	Internal Representation	Spectral Cells Formation

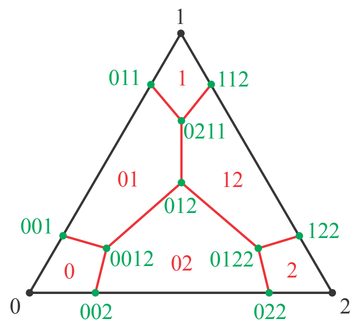
Order 2



Spectral Cell

id	v_1	v_2	v_3	v_4
0	0	02	012	01
1	1	01	012	12
2	2	12	012	02

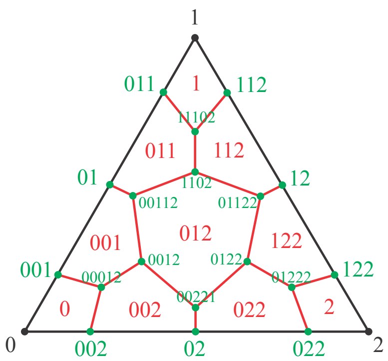
Order 3



Spectral Cell

id	v_1	v_2	v_3	v_4	v_5
0	0	002	0012	001	
1	1	011	0211	112	
2	2	122	0122	022	
01	001	0012	012	0211	011
12	112	0211	012	0122	122
02	002	022	0122	012	0012

Order 4



Spectral Cell

id	v_1	v_2	v_3	v_4	v_5	v_6
0	0	002	00012	001		
1	1	011	11102	112		
2	2	122	01222	022		
001	001	00012	0012	00112	01	
011	01	00112	1102	11102	011	
112	112	11102	1102	01122	12	
122	12	01122	0122	01222	122	
022	02	022	01222	0122	00221	
002	002	02	00221	0012	00012	
012	00221	0122	01122	1102	00112	0012

Figure 3. Internal representation of spectral volumes.

5.1 Wedge flow

In this experiment, we simulated a supersonic flow (mach number $M_1 = 2.5$) past a wedge with half-angle of 15 degrees. The shock angle β is given as $\beta = 36.94$. The leading edge is located at coordinates $x = 0$ e $y = 0$. The inlet boundary is located in $x = -0.5$, and the outlet in $x = 1.0$. The farfield boundary is located in y=1.0.

The mesh that was used in the experiments has 2360 nodes and 4524 volumes. The first test was performed with the spectral schemma of order two. The mesh partitioning using this order can be viewed in Fig. 4, together with a zoom at the indicated mesh region. showing the cells division made in internal elements of each spectral volume. The new mesh has 13767 nodes and 13572 volumes.

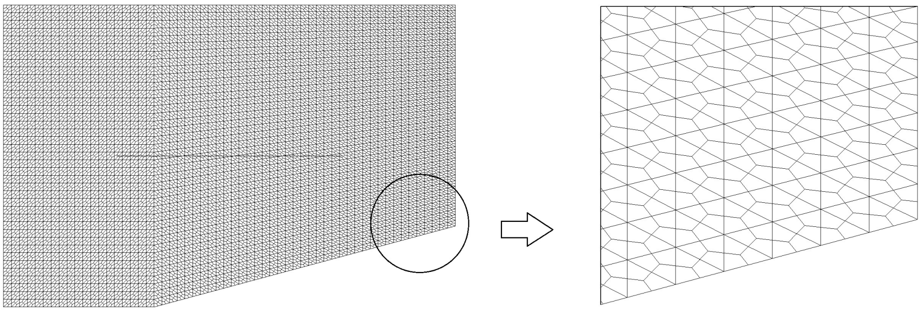
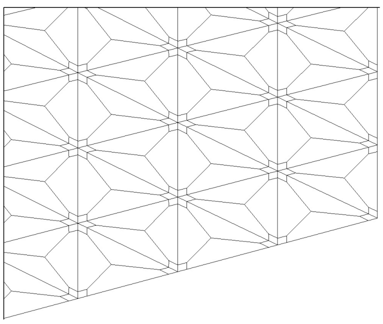
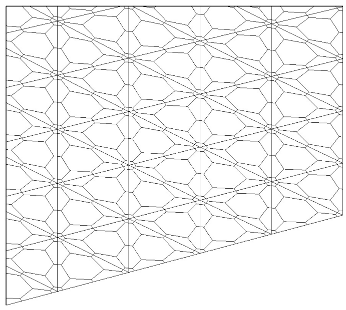


Figure 4. Mesh generated by the spectral finite volume method of second order.

The second and third test were done by using spectral schemes of order 3 and 4, respectively. A sample of the mesh partitioning results for this cases can be seen in Fig. 5(a) and 5(b). It can be seen in the zoom areas the different partitioning done by each case. The result mesh for third order of precision has 34222 nodes and 27144 volumes, while the fourth order mesh has 63725 nodes and 45240 volumes.



(a) Third order



(b) Fourth order

Figure 5. Mesh samples generated by the spectral finite volume method.

The Figure 6 shows the residue history in the first 5000 iterations of both implementations, for all precision order schemes used in the experiments. It can be seen that the fourth order precision method presented the better convergence rate in the tests.

The plots showed in Figure 7 show the distribution of pressure coefficient (Cp) over the wedge surface compared with the analytical solution already known Anderson (1990), for both implementations. In the Fig. 7(a) is shown the Cp for the second order schema, while Fig. 7(b) and 7(c) show the Cp for the third and fourth order method, respectively. From the results, we can note that the precision method of fourth order produces better results from the other precision orders, taking as parameter the proximity with the analytical solution. One possible interpretation is that the fourth order resulted in a better mesh partitioning, along with a higher number of nodes and cells, allowing to identify more details of the numerical simulation.

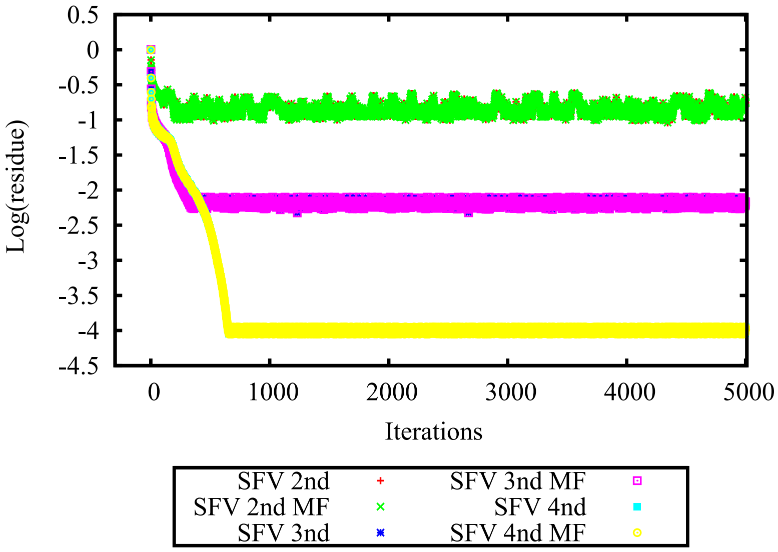
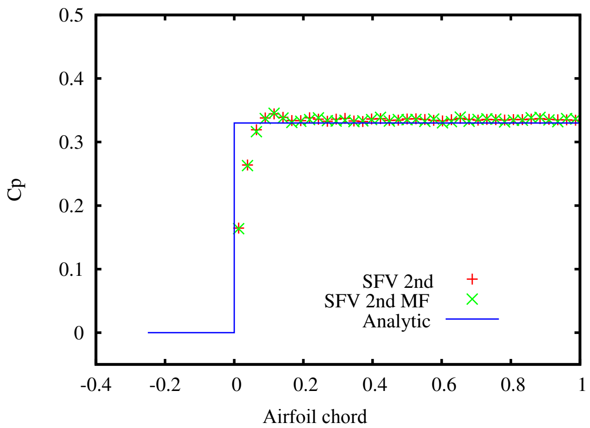
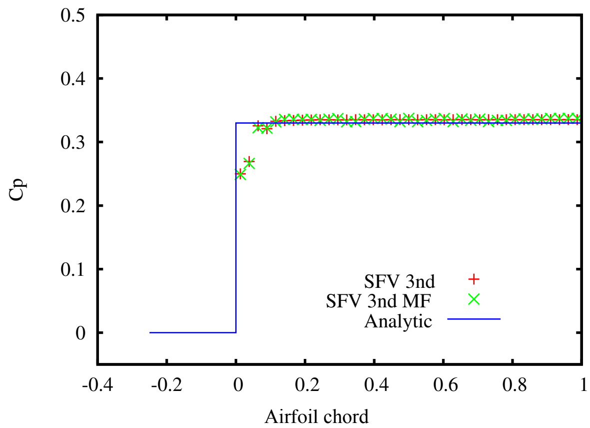


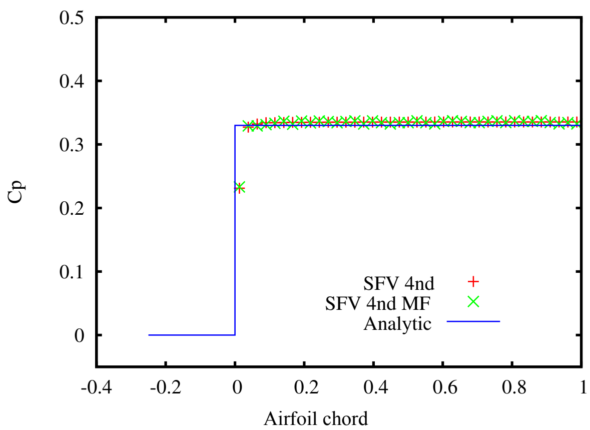
Figure 6. Residue history for all tested schemes.



(a)



(b)



(c)

Figure 7. Plots of pressure distribution coefficient for the precision order methods, (a) second precision order, (b) third precision order and (c) fourth precision order.

6. CONCLUSION

In this paper we presented an approach do extend an existing data structure to be able to index elements created by the spectral finite volume method. We showed a mapping procedure that covers the indexing of elements generated by the second up to the forth order of precision of the spectral finite volume method.

Each precision order provides different configuration of the partitioned mesh, with a different number of elements formed. We presented the general formulation of the spectral volume method and provided the specifics for the indexing adaptation on the chosen data structure.

Experiments shown the validation of our indexed technique over a non-indexed implementation. Results showed a good approximation of the results. Future works in this field include computational measures for performance of simulations by using indexed meshes, where a better memory usage and mesh access is provided by using such data structures.

7. ACKNOWLEDGEMENTS

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9. RESPONSABILITY NOTICE

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