ONERA

THE FRENCH AEROSPACE LAB

www.onera.fr

PROPOSITION DE SUJET DE THESE

Title : Extension of a high-order Spectral Difference method to mixed-element grids with application to LES of a combustion chamber

Référence : **SNA-DMPE-2024-30**
(à rappeler dans toute correspondance)

PhD Start date : October 2024	**Deadline for applications :** end of June 2024

Keywords : LES, combustion, mixed-element grids, high-order

Candidate Profile:

Good knowledge of numerical methods, fluid dynamics of reacting and non-reacting flows, turbulent combustion and LES. Good programming and communication skills. Ability to work in a team.

Presentation of PhD topic, context and main goals:

The need for accurate and efficient numerical simulations in the aeronautics and aerospace industry has considerably increased in recent years. The aim is to reduce the development costs by gradually replacing expensive experimental tests with cheaper and more flexible numerical simulations. Improving the performance of propulsion systems in aircrafts, helicopters, and rockets is in fact a major challenge. In this context, the use of Large-Eddy Simulation (LES) in combination with high-order accurate numerical schemes appears to be essential. In this line of research, ONERA and CERFACS are currently working in close collaboration with the aim of developing innovative computational methods within the JAGUAR high-order CFD solver.

JAGUAR solves the reacting Navier-Stokes equations in the turbulent flow regime by means of LES on unstructured quadrilateral or hexahedral grids. The numerical discretization of the equations is based on a high-order Spectral Difference (SD) method, which is part of the larger family of discontinuous spectral methods. In the SD framework, the solution in each cell is expressed as a polynomial of given degree p, which determines the order of the method (p+1). A major advantage of the SD method is that the solution is allowed to be discontinuous across interfaces of adjacent cells, making this type of method particularly well suited to parallel implementations.

During the PhD thesis by A. Veilleux, the SD method originally implemented in JAGUAR has been extended to triangles [2], up to p=5, and to tetrahedra [1], currently limited to p=2. The PhD work of T. Marchal [3] has made it possible to perform reacting flow simulations using JAGUAR on hexahedral meshes based on the standard SD scheme. On a different line of research, a new version of the SD method, which makes the scheme stable in the presence of a discontinuity [4], has recently been developed.

Main objectives of the PhD thesis:

The main goal of the PhD thesis proposed here is thus to continue these efforts and to go beyond the state of the art of high-order discontinuous spectral methods by improving and extending the capabilities of the JAGUAR solver to deal with reacting flow configurations of practical interest to the aeronautics and aerospace industry [5]. The target application is the PRECCINSTA reacting flow configuration [3] on a hybrid mesh composed of tetrahedra and prisms.

First line of research: extension of previous work to hybrid meshes.

The formal development of a stable SD formulation on prisms was carried out in the framework of the thesis of A. Veilleux [2], who proposed a stable formulation of the SD scheme on triangles up to 6-th order (p=5). This new formulation is based on a tensor product of the 2D SD scheme on triangles and a 1D reconstruction in the other direction. Even though the theoretical formalism has already been laid out, its practical implementation into JAGUAR has not yet been carried out. To do so, it will be necessary to modify the solver so that it can read and process meshes, first solely composed of prisms, then hybrid meshes composed of both prisms and tetrahedra. The solver kernel, and in particular the diffusive scheme and the non-reflecting boundary conditions, will then have to be revisited in order to take into account prismactic and tetrahedral grids. These new developments will be validated on academic configurations (e.g. convection of an isentropic vortex, Taylor Green Vortex…).

Second line of research: stable SD formulation on tetrahedra at higher order (p > 2).

Achieving a stable formulation on tetrahedra requires a particular placement of certain points in the volume and on the faces of the tetrahedra. We have imposed the position of these points on the faces and we have parameterized the position of the flux points in the interior of the cells. Thanks to an optimization algorithm, a stable formulation for polynomials of degree 1 and 2 has been derived, which guarantees an order of 2 and 3, respectively. However, we did not succeed in obtaining a stable higher-order formulation on tetrahedra. To achieve this, we can consider several solutions. The obvious extension of the previous work consists in finding the optimal position of both the internal flux and boundary points by using the optimization algorithm. Another more involved approach would be to revisit the polynomial approach proposed by Raviart and Thomas as regards the polynomial representation of the flux function. Once a new stable formulation is achieved, it will be implemented and validated on the linear advection problem and the isentropic vortex configuration. The work carried out on prisms and tetrahedra as regards the diffusive scheme will allow us to quickly implement the approach into the solver. After validation in a non-reacting flow configuration, we will focus on reacting flow computations on tetrahedral meshes.

Finally, the PRECCINSTA reacting flow configuration [3] on a hybrid mesh composed of tetrahedra and prisms will be used to assess the performance of the proposed high-order SD approach.

The outcome of this research will lead to a number of publications in the field of numerical methods (Journal of Computational Physics, Journal of Scientific Computing, etc.) and combustion (Combustion and Flame, etc.).

Bibliography :

[1] Veilleux, A., Puigt, G., Deniau, H. and Daviller, G. (2022) Stable Spectral Difference Approach Using Raviart-Thomas Elements for 3D Computations on Tetrahedral Grids, *Journal of Scientific Computing*, 91, 7

[2] Veilleux, A., Puigt, G., Deniau H. and Daviller, G. (2022), A stable Spectral Difference approach for computations with triangular and hybrid grids up to the 6th order of accuracy, *Journal of Computational Physics*, 449, pp. 110774, 2022

[3] Marchal, T. and Deniau, H. and Boussuge, J.-F. and Cuenot, B. and Mercier, R. (2021) *Extension of the Spectral Difference method to combustion.* arXiv preprint arXiv:2112.09636

[4] Deniau H. and Puigt G., Entropy stable spectral difference scheme, H. Deniau and G. Puigt, *European workshop on high order nonlinear numerical methods for evolutionary PDEs: theory and applications (HONOM2022)*, April 4-8, Braga, Portugal, 2022.

[5] Gicquel, Laurent and Staffelbach, Gabriel and Poinsot, Thierry (2012) *Large Eddy Simulations of gaseous flames in gas turbine combustion chambers.* Progress in Energy and Combustion Science, vol. 38 (n° 6). pp. 782-817. ISSN 0360-1285

[6] https://www.theses.fr/2021INPT0029/document

[7] Fiévet, R., Deniau, H., Piot, E., Strong compact formalism for characteristic boundary conditions with discontinuous spectral methods, Journal of Computational Physics, 408, 1 May 2020, pp. 109276

Collaborations envisages	
The Ph.D. is funded jointly by ONERA/CERFACS. Many travels between ONERA and CERFACS are planned during the Ph.D. and both centers are located in Toulouse.	
Laboratoire d'accueil à l'ONERA Département : Département Multi-Physique pour l'Energétique Lieu (centre ONERA) : Toulouse **Contact** : Marta De La Llave Plata, Hugues Deniau et Guillaume Puigt Tél. : 0562252940 Email : Marta.De_La_Llave_Plata@onera.fr, Hugues.Deniau@onera.fr,	**Directeur de thèse** Nom : Guillaume PUIGT (ONERA) et Guillaume Daviller (CERFACS) Laboratoire : ONERA/DMPE et CERFACS Tél. : 0562252940 Email : Guillaume.Puigt@onera.fr

Pour plus d'informations : https://www.onera.fr/rejoindre-onera/la-formation-par-la-recherche