A massively parallel solution strategy for efficient thermal radiation simulation

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Abstract. A novel and efficient methodology to solve the Radiative Transfer Equations (RTE) in thermal radiation is discussed. The BiCGStab(2) iterative solution method, as designed for the non-symmetric linear equation systems, is used to solve the discretized RTE. The numerical upwind and central schemes are blended to provide a stable numerical scheme (MUCS) for interpolation of the cell facial radiation intensities in finite volume formulation. The combination of the BiCGStab(2) and MUCS methods proved to be very efficient when coupling with the DOM approach to solve the RTE. A cost-effective tabulation technique for the gaseous radiative property model SNB-FSCK using 7-point Gauss-Labatto quadrature scheme is also introduced. The whole methodology is implemented into a massively parallel unstructured CFD code where the radiative and fluid flow solutions share the same domain decomposition, which is the bottleneck in current radiative solvers. The dual mesh decomposition at the cell groups level and processors level is adopted to optimize the CFD code for massively parallel computing. The whole method is applied to simulate the radiation heat-transfer in a 3D rectangular enclosure containing non-isothermal CO₂ and H₂O mixtures. Two test cases are studied for homogeneous and inhomogeneous distributions of CO₂ and H₂O in the enclosure. The result is reported for the heat flux and radiation energy source and the comparison is also made between the present methodology BiCGStab(2)/MUCS/tabulated SNB-FSCK, the benchmark method SNB-CK (implemented at 25cm⁻¹ narrow-band) and some other methods available in the literature. The present method (BiCGStab(2)/MUCS/tabulated SNB-FSCK) yields more accurate predictions particularly for the radiation source term. When comparing with the benchmark solution, the relative error of the radiation source term is remarkably reduced to less than 4% and the CPU time is drastically diminished.

1. Introduction
The success in the design of advanced combustion systems relies heavily on accurate and efficient CFD solvers, combustion and heat transfer modeling. In the latter, thermal radiation occupies a large portion in the total balance of heat transfer. Recent developments of Modest [1] and Liu et al [2] in global gas radiative modeling gave birth to the Statistical Narrow Band Full Spectrum Correlated K

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(SNB-FSCK) model which is a compromise between the solution accuracy and computational effort if one compares with the standard band SNB-CK model (accurate but less efficient) [3] and with the global Weighted-Sum-of-Gray-Gases (WSGG) model (efficient but less accurate) [4]. The SNB-FSCK model can be implemented into radiative solvers in its expensive on-line calculation or in its pre-computation or tabulation version [2][5][6]. Nevertheless, the level of the computational accuracy and efficiency of the SNB-FSCK model is dependent on the way one couples the model with solution methods for the RTE. The tabulated SNB-FSCK model that can be used in an accurate way to gain in efficiency will be explored in the present study.

The Discrete Ordinate Method (DOM) [7] is presently one of the most widely used solution methods for discretizing the Radiative Transfer Equation (RTE) in directions because it ensures a good compromise between solution accuracy and computational cost in many practical applications [8]. This method combined with the Finite Volume (FV) discretization is particularly adapted to practical applications with complex geometry because it can be used with non-structured grids [6]. The DOM is suited to be used along with the CK and global gas radiative property models (WSGG, SLW, ADF, FSK) [8], and recently with the SNB-FSCK model. The Exponential [9], Step [10] and Diamond Mean Flux Schemes (DMFS) [11] are the conventional numerical schemes for solving the RTE, but many other schemes categorized under the Normalized Variable Diagram (NVD), Total Variation Diminishing (TVD), Essentially Non-Oscillatory (ENO), Genuinely multidimensional schemes families are also available [12,13]. However, concerning the methods to handle the RTE for unstructured grids in complex geometries, this is still a challenging task and very little work has been done to date in this direction. A sweeping optimization technique [6] was used to reorganize the cell faces numbering according to radiation wave propagation direction. The technique itself is intrinsically a serial process and the paralleling computing was carried out based on splitting the number of discrete directions. In some cases, the calculations of the emission and absorption terms had to be split into different processors. This method of paralleling is completely decoupled from the spatial domain decomposition used in CFD and would be limited when dealing with massively parallel computation. Santos et al. [14] developed a methodology to couple a LES solver with a radiation code, but the two codes didn’t use the same computational domain; the LES solver was parallelized by domain decomposition whereas the radiation code was based on optical rays and was parallelized by splitting in the spectral domain. An additional data exchange protocol was needed to ensure the coupling between the two codes, the computational cost was still very heavy (two-thirds of processors for radiative solver and one-third for combustion solver) and the simulation was limited to 2D cases [14].

To overcome these difficulties, a new methodology is proposed in this study to solve the RTE in the same computational grid mesh with CFD solver. In this light, the BiCGStab iterative solution method [15] is adapted to solve the non-symmetric linear equation system resulting from discretizing the RTE. It should be noted that the variant BIGSTAB was used in a parallel unstructured CFD code [16] for radiation calculation. Concerning the numerical scheme used to interpolate the cell facial radiation intensities, the Upwind scheme is blended with the Central scheme to give a stable scheme with limited dispersion and dissipation, called Mixed Upwind and Central Scheme (MUCS). According to the authors’ acknowledge, it is the first time that the tabulated SNB-FSCK method, the MUCS scheme and the BiCGStab iterative solution method are combined and implemented in an unstructured code to calculate thermal radiation. The advantage of this method is that the radiative and CFD solvers share the same domain decomposition and parallelism and they are coupled in a natural manner needing no correction for load balancing or no adjustment on the number of cores devoted to each solver as done in [14]. This is paving the way for coupling radiative transfers with turbulent combustion for practical systems in the context of massively parallel computing as the solver used in the study has proved to be successful in simulating a semi-industrial swirl burner with a mesh of 2.6 billion cells [17].
The section below describes the methodology of combining the MUCS scheme and the BiCGStab iterative solution methods to solve the non-symmetric linear system of the discretized RTE with some specific care for boundary treatment. In the next section, the devised methodology is employed to calculate the thermal radiation within a 3D enclosure and the simulation results are compared with other methods presented in the work of Liu et al. [2] with emphasis on solution accuracy and computational efficiency of our radiative solver. Finally, conclusions will be drawn out.

2. Methodology

The discretization of the RTE proceeds through three steps: discretization in frequency, discretization along propagation directions of radiation beams, and discretization in space within computational domain. The discretization in frequency which is particularly related to the SNB-FSCK method is presented in [1,2]. The 7-point Gauss-Labatto quadrature scheme [2] is used in the study to pre-define the discretization points in the cumulative distribution \( g \)-space for the RTE. The DOM/S4 [18] is used in the study for the direction discretization because of a good compromise between solution accuracy and computational requirements in practical calculations of combustion systems. The discretization of the RTE in space is carried out by using the Finite Volume method in the context of unstructured mesh based applications. The upwind and central schemes are blended and an iterative solver is used for inverting the non-symmetric linear system resulting from the discretization of the RTE. These methods, with special care about the specific boundary handling for this problem, are developed together in the following. The RTE in the cumulative distribution \( g \)-space to be solved can be rewritten in the form [1,2]:

\[
s \cdot \nabla I_g = -k^* I_g + k^* a I_b
\]

where \( I_g \) (W/m) is the radiation intensity in the \( g \)-space, \( I_b \) (W/m) the blackbody radiation intensity, \( k^* \) (m\(^{-1}\)) the full spectrum absorption coefficient, \( a \) the weight function. This equation will be integrated over a node-centered control volume \( V_i \) (see Figure 1.a) using the Gauss’ theorem:

\[
\sum_{j=1}^{N_{sec}} A_j (n_j \cdot s) I_{g,j} + k^* V_i I_{g,i} = (k^* a I_b)V_i
\]

where \( n_j \) is the outward unit normal to the face \( j \), \( A_j \) is the area of the face \( j \), \( i \) denotes the node \( i \), and \( V_i \) is the node-centered control volume at node \( i \). Figure 1.a shows an illustration of the finite volume discretization; one can see, for example, that \( V_i \) is the volume bounded by the dash lines.

**Figure 1.** (a) Illustration of the MUCS scheme. (b) Illustration of the boundary treatment.
To close Equation (2), i.e., to calculate the nodal radiation intensity \( I_{g,j} \), one needs to express the radiation intensities on the control volume surfaces \( I_{g,k} \) in term of the nodal radiation intensity \( I_{g,j} \).

We propose an alternative to the conventional schemes (Exponential [9], Step [10], DMFS [11], NVD, TVD, ENO, Genuinely multidimensional [12,13]) to solve the RTE. The alternative is the BiCGStab iterative solution method combined with the stable Mixed Upwind and second-order Central Scheme (MUCS). In the framework of kinetic-energy conserving discretization in finite volume method [19], the second-order central scheme (CS) can be blended with the Upwind Scheme (US) to give a scheme which possesses the advantages of the two mother schemes such as being close to second-order accuracy, limiting the intensity diffusion and keeping the intensity bounds. The MUCS scheme is expressed in the form:

\[
I_{g,j} = \begin{cases} 
\gamma^j I_{g,j} + (1 - \gamma)(I_{g,j} + I_{g,k})/2 & \text{if } D_j > 0 \\
\gamma^j I_{g,k} + (1 - \gamma)(I_{g,j} + I_{g,k})/2 & \text{if } D_j \leq 0 
\end{cases}
\]  

(3)

where \( D_j \) is the scalar product between the unit vector of the discrete direction \( s \) and the normal to the face \( j (n_j) \). The blending factor \( \gamma, 0 \leq \gamma \leq 1 \), determines how much numerical diffusion of the upwind scheme is introduced. The value of \( \gamma = 0.2 \) led to a low-dispersion MUCS scheme and therefore is adopted in the study. The BiCGStab(2) method [15], as designed for the non-symmetric linear equation systems, is adopted in the study and consists in solving the following linear system:

\[
Ax = b
\]  

(4)

The discretized RTE of Equation (2) can be transformed in the form of Equation (4). \( b \) is the Right Hand Side (RHS) of the linear system and corresponds to the emission term, i.e., \( b = (k^*a \cdot I_0) V_I \). This emission term depends on local radiative properties and is known prior to the solving of the linear system. \( Ax \) is the Left Hand Side (LHS) of the linear system and contains two terms: the propagation term \( \sum_{j=1}^{N_{\text{faces}}} A_j(n_j \cdot s)I_{g,j} \) and the absorption term \( k^*V_I I_{g,j} \). \( x \) is a vector of unknowns \( I_{g,j} \) (after expressing \( I_{g,j} \) in term of \( I_{g,j} \) using the MUCS scheme). The matrix \( A \) is always non-symmetric whatever the blending factor \( \gamma \) is.

The cell elements having faces lying on the boundary should be handled properly in the iterative solution method. The solution consists in considering two situations according to the sign of the scalar product between the unit vector of the discrete direction \( s \) and the normals to the face lying on the boundary \( (n_{in} \text{ and } n_{out}) \), as shown in Figure 1.b. \( D_{\text{out}} = s \cdot n_{out} > 0 \): the boundary radiation in this direction is calculated from the radiation obtained in the cell volume adjacent to the boundary, so the boundary radiation is an unknown, therefore the boundary propagation term \( A_j(n_j \cdot s)I_{g,j} \) is kept in \( Ax \) of Equation (4), i.e., on the LHS of the linear system. \( D_{\text{in}} = s \cdot n_{in} \leq 0 \): the boundary radiation in this direction is calculated from the radiation known on this boundary. This corresponds to the application of the Dirichlet condition and therefore the boundary propagation term \( A_j(n_j \cdot s)I_{g,j} \) is sent to the RHS of the linear system (Equation (4)). The whole methodology is implemented into the massively parallel unstructured CFD code called YALES2 [17], where the radiative and fluid flow solutions share the same domain decomposition, which is the bottleneck in current radiative solvers. The dual mesh splitting at the cell groups level and processors level is used to optimize the CFD code for massively parallel computing.
As the online calculation of the full spectrum absorption coefficient \( k^* \) can consume a large amount of CPU time in thermal radiation calculations, it is preferable to pre-compute \( k^* \) prior to solving the RTE [2,6]. In this way, the absorption coefficient \( k^* \), the weight function \( a \), and the blackbody radiation intensity \( I_b \) are calculated first in function of temperature, molar fractions of CO\(_2\) and H\(_2\)O. This allows for the tabulation of the absorption coefficient \( k^* \) and the emission term \( k^*aI_b \), for 7 Gauss-Labatto quadrature points, as functions of three indices: temperature \( T \), molar fraction of CO\(_2\) and H\(_2\)O \( (X_{CO_2}, X_{H_2O}) \). A multi-dimensional linear interpolation method is implemented to interpolate \( k^* \) and \( k^*aI_b \) at the actual local state \( (T, X_{CO_2}, X_{H_2O}) \) of the mixture during the simulation. It should be noted that, the method for tabulating \( k^* \) and \( k^*aI_b \) used in the present study is different from the \( k^* \) pre-calculation method in the work of Liu et al. [2]. In fact, Liu et al. [2] used the 4-point Gauss quadrature scheme and the values of \( k^*_{CO_2} / pX_{CO_2} \) and \( k^*_{H_2O} / pX_{H_2O} \) were calculated and fit to a 9th-order polynomial function of \( T \) varying between 300 K and 2600 K for a range of reference temperatures \( T_0 \) between 500 K and 1600 K with intervals of 100 K. A 1D linear interpolation was employed to obtain the radiative properties at the actual reference \( T_0 \). The radiative property database from Soufiani and Taine [20] together with the approximate Malkmus band method [21] appear to be an appropriate strategy to calculate the mixture property, as follows:

\[
\begin{align*}
\frac{k^2_{\Delta \nu, \text{mix}}}{\Phi_{\Delta \nu, \text{mix}}} = & \frac{k^2_{\Delta \nu, CO_2}}{\Phi_{\Delta \nu, CO_2}} + \frac{k^2_{\Delta \nu, H_2O}}{\Phi_{\Delta \nu, H_2O}} \\
\frac{k_{\Delta \nu, \text{mix}}}{\Phi_{\Delta \nu, \text{mix}}} = & \frac{k_{\Delta \nu, CO_2}}{\Phi_{\Delta \nu, CO_2}} + \frac{k_{\Delta \nu, H_2O}}{\Phi_{\Delta \nu, H_2O}}
\end{align*}
\]

(5)

where \( k_{\Delta \nu, \text{mix}} \) \((m^{-1})\) is the average absorption coefficient of the mixture over a narrow band \( \Delta \nu \), \( \Phi_{\Delta \nu, \text{mix}} \) (dimensionless) is the average line width to spacing ratio of the mixture. \( k_{\Delta \nu, \text{mix}} \) and \( \Phi_{\Delta \nu, \text{mix}} \) are SNB model parameters to calculate the full-spectrum mixture absorption coefficient \( k^* \) that depends on local temperature and partial pressure, i.e., mole fractions of radiating gases and also on the reference state of the mixture. The reference state of the mixture can be chosen beforehand; Liu and Smallwood [5] proposed to choose the reference mixture consisting of \( X_{CO_2,0} = 0.1 \) and \( X_{H_2O,0} = 0.2 \) and the reference temperature can be calculated using the volume averaged temperature formulation proposed by Modest and Zhang [22] such as:

\[
T_0 = T_{ref} = \frac{1}{V} \int_T V T dV
\]

(6)

3. Results and discussion

3.1. Configuration of the test case

The configuration for the test is a 3D rectangular enclosure as used in the works of Liu et al. [2] and of Liu and Smallwood [5]. The test case simulates a water-cooled gas-fired furnace. The enclosure has 2m in x, 2m in y and 8m in z and is divided into 17(x).17(y).40(z) = 11560 cell volumes with regular grid distribution in three directions. The number of cell volume is kept as the same used in the work of Liu et al. [2] for comparison purpose. The mixture contained in the enclosure consists of CO\(_2\), H\(_2\)O and N\(_2\) under 1atm pressure. The non-uniform distribution of temperature is specified as
where \( T_{\text{axis}} \) and \( f(r) \) define the temperature distribution along the centerline and radial direction, respectively, with

\[
T_{\text{axis}} = \begin{cases} 
0\text{ if } 0 \leq z < 0.75 \text{ m} \\
800 + (2100 - 800)(8 - z) / 7.25 \text{ if } 0.75 \text{ m} \leq z \leq 8 \text{ m}
\end{cases}
\]

and \( f(r) = 1 - 3r^2 + 2r^3 \), where \( r \) is the distance to the centerline. In the four corner regions where \( r > 1 \text{ m} \), \( T \) simply takes the value of temperature evaluated at \( r = 1 \text{ m} \). Temperature is expressed in Kelvin. Equation (6) can be now applied and it yields the reference temperature \( T_0 = 948.48 \text{ K} \). In the following sections, we present the result of the calculations for two cases: homogeneous and inhomogeneous distributions of CO\(_2\) and H\(_2\)O. The result consists of wall heat flux and radiation source term. To validate our methodology, the present result will be compared to that obtained by Liu et al. [2] in the same configuration. The result of Liu et al. [2] marked by SNB-CK is used as the benchmark solution, the SNB-FSCK/M1 and SNB-FSCK/M2 methods used the on-line inversion and the pre-computation of the full spectrum absorption coefficient \( k^* \), respectively, and the SNB-CK/9band employed the optimized 9-band model. Liu et al. [2] used the same 7-point Gauss-Labatto quadrature scheme for the benchmark solution while the 4-point Gauss quadrature scheme was used for other methods.

3.2. Homogeneous distribution of CO\(_2\) and H\(_2\)O

In this case, the mole fractions of CO\(_2\) and H\(_2\)O take values of \( x_{\text{CO}_2} = 0.1 \) and \( x_{\text{H}_2\text{O}} = 0.2 \), and are the same everywhere inside the enclosure. Figure 2 shows the contour of radiative heat source in the Oxz plane. Because the mole fraction distributions of CO\(_2\) and H\(_2\)O are uniform, the contour of radiative source term basically follows the pattern of the temperature contour (not shown here). The mixture radiates the most in the region of high temperature around \( z = 0.775 \text{ m} \) along the centerline. The negative and positive values of the radiation source term indicate the heat loss and gain, respectively, due to the radiative heat transfer. In the parietal regions, the gases absorb the heat emitted from the central region.

Figure 3 shows the evolution of the wall heat flux along the center of the side wall and the radiation source term along the centerline of the enclosure. In the same figure, the results of the present method BiCGStab(2)/MUCS/tabulated SNB-FSCK, denoted by SNB-FSCK/MUCS, are compared with those from Liu et al. [2]. Concerning the distribution of the wall heat flux shown in Figure 3.a, the present result (SNB-FSCK/MUCS) is generally better than the result using the SNB-FSCK/M2 method in Liu et al. [2]. The relative error measured between the present method (SNB-FSCK/MUCS) and the SNB-CK benchmark at the maximum absolute values of the wall heat flux reduces to 7% as compared to 15% resulting from the comparison between the SNB-FSCK/M2 method and the SNB-CK benchmark. This amelioration lies in the more efficient tabulation method, the use of the Malkmus band to handle the spectral properties of the mixture and of the 7-point Gauss-Labatto quadrature scheme in the present study. In Liu et al. [2], the absorption coefficients were calculated by making the assumption on the correlation of CO\(_2\) and H\(_2\)O radiative properties. This assumption yields large error for the mixture absorption coefficient.

Another very interesting result is obtained when one observes the distribution of the radiation source term as shown in Figure 3.b. The result of the present method (SNB-FSCK/MUCS) is in very good agreement with that of the benchmark SNB-CK. At the maximum absolute values of radiation source term, the present method (SNB-FSCK/MUCS) produced less than 4% of error as compared to 14% resulted from the SNB-FSCK/M2 method. The present method (SNB-FSCK/MUCS) gives a similar result with the SNB-FSCK/M1 and SNB-CK/9band methods but with a computational time largely
reduced, as shown later in the paper. It can be seen that the present method (SNB-FSCK/MUCS) exhibits an advantage over the SNB-FSCK/M1, SNB-FSCK/M2 and SNB-CK/9band methods.

3.3. Inhomogeneous distribution of CO₂ and H₂O

In the second test, the mole fraction of CO₂ and H₂O are linear in z-direction and kept uniform in x and y directions. The distributions of CO₂ and H₂O along the z-direction are given as follows:

\[
X_{CO_2} = \begin{cases} 
0.6z & \text{if } 0 \leq z \leq 0.5 \text{ m} \\
(-0.25z + 2.375)/7.5 & \text{if } 0.5 \text{ m} < z \leq 8 \text{ m}
\end{cases}
\]  \hspace{1cm} (8)

\[
X_{H_2O} = \begin{cases} 
z & \text{if } 0 \leq z \leq 0.5 \text{ m} \\
(-0.45z + 3.975)/7.5 & \text{if } 0.5 \text{ m} < z \leq 8 \text{ m}
\end{cases}
\]  \hspace{1cm} (9)

Similarly to the homogeneous test case, Figure 4 shows the evolution of the wall heat flux along the center of the side wall and the radiation source term along the centerline of the enclosure. For the wall heat flux, the present method (SNB-FSCK/MUCS) shows the result which is practically equivalent to that obtained with the SNB-FSCK/M2 method (Figure 4.a). The relative error between the present method (SNBFSC/MUCS) and the SNB-CK benchmark at the maximum absolute values of the wall heat flux is 12% as compared to 11% resulted from the comparison between the SNBFSC/M2 method and the SNB-CK benchmark. We can see again, from the result of the radiation source term
shown in Figure 4.b, that the present method (SNB-FSCK/MUCS) is in a very good agreement with the SNB-CK benchmark. At the point of maximum absolute values of the radiation source term, the relative error between the present method (SNB-FSCK/MUCS) and the benchmark method SNB-CK is reduced to less than 4% as compared to 18% resulted from the SNB-FSCK/M2 and SNB-CK comparison. The present method (SNB-FSCK/MUCS) predicts the radiation energy source much better than the SNBFSCK/M2 in a large portion of the enclosure and also better than the SNB-CK/9band in the region of high absolute values of the radiation energy source.

Figure 4. Inhomogeneous case. (a) Wall heat flux along the center of the side wall, (b) Radiation source term along the centerline of the enclosure. Triangle: present method BiCGStab(2)/MUCS/tabulated SNB-FSCK; circle: benchmark correlated K model; line: SNB-FSCK with on-line inversion of $k^*$; dashed-line: SNB-FSCK with pre-computation of $k^*$; dotted-line: optimized 9-band SNB-CK model.

3.4. Computational efficiency and accuracy

CPU times are compared in Table 1 to indicate the efficiency of the method developed in the present study. However, this should not be taken as an exact comparison because the present calculations and those of Liu et al. [2] were performed on different computers. The present calculations were carried out on IDRIS-CNRS computing resources (Vargas computer: IBM SP Power6, 3584 processors, 18 Tbytes, 68 Tflops) [23] while those of Liu et al. [2] on a Pentium 4 2.8 GHz PC. The computational times of runs using one processor are reported in Table 1 for comparison.

It is clearly noted that the CPU time of the present method (SNB-FSCK/MUCS) is significantly lower than that of the benchmark method SNB-CK by a factor of about 368 which is the expected CPU time reduction because we reduced the number of narrow bands from 367 to 1 global band, indicating the excellent efficiency of the new method. The CPU time of the present method (SNB-FSCK/MUCS) is systematically lower than that of the SNB-FSCK/M1 method (a factor of about 6), that of the SNB-FSCK/M2 method (a factor of about 1.2) and that of the SNB-CK/9band method (a factor of about 3.4). Three important points should be noted to understand the superiority of the SNB-FSCK/MUCS method. The first point is that the present method (SNB-FSCK/MUCS) used the 7-point Gauss-Labatto quadrature scheme for a better description of the gas radiative properties as compared to the 4-point Gauss quadrature scheme used in the SNB-FSCK/M1 and SNB-FSCK/M2. The second point is that the present method (SNB-FSCK/MUCS) is implemented into an unstructured software designed for complex geometries and it is known that an unstructured code needs about four times longer than a structured code and this constitutes a very important advantage of the present method. The third point is that the present method (SNB-FSCK/MUCS) can predict the radiation source term with more accuracy than other methods with less CPU times spent.
It should also be noted from Table 1 that, the first-order accuracy Upwind scheme (US) even reduced the calculation time down to nearly one and a half times if we compare with the MUCS scheme (i.e., 24.7s compared with 16.9s). However, this efficiency was obtained at the expense of accuracy. Figure 5 shows indeed the comparison between the MUCS and US schemes for the wall heat flux and radiation source term in the homogeneous case. It is clear from this figure that the MUCS scheme gives much accurate results than the US scheme when comparing to the SNB-CK benchmark. The radiative solver runs massively in parallel and as one example of this, 1024 processors of Vargas machine [23] were used to calculate the same configuration with 24 million of cells for the homogeneous distributions of CO₂ and H₂O. The corresponding computational time is 560.5s and the result of the parallel run is also presented in Figure 5.

| Method                  | No. of quadrature points | No. of bands | CPU time (s) |
|-------------------------|--------------------------|--------------|--------------|
| SNB-FSCK/MUCS           | 7                        | 1            | 24.7         |
| SNB-FSCK/US             | 7                        | 1            | 16.9         |
| SNB-CK(*)               | 7                        | 367          | 9086.3       |
| SNB-FSCK/M1(*)          | 4                        | 1            | 146.9        |
| SNB-FSCK/M2(*)          | 4                        | 1            | 30.7         |
| SNB-CK/9band(*)         | 4                        | 9            | 84.91        |

(*)Results of Liu et al. [2]

Figure 5. Homogeneous case. Comparison of accuracy between the US and MUCS schemes and results of massively parallel run (marked with dashed line). (a) Wall heat flux along the center of the side wall; (b) Radiation source term along the centerline of the enclosure. Circle: benchmark correlated K; triangle-up: BiCGStab(2)/MUCS/tabulated SNB-FSCK with 11560 cells (monoprocessor); dashed-line: BiCGStab(2)/MUCS/tabulated SNB-FSCK with 24 million cells (1024 processors); triangle-down: BiCGStab(2)/US/tabulated SNB-FSCK with 11560 cells (monoprocessor).

4. Conclusion
A new method to solve the RTE in radiation problems is introduced in the present study. The second-order central and first-order upwind schemes are blended to give a stable numerical scheme (MUCS). The BiCGStab(2) iterative solution method is used to solve the non-symmetric linear system of the discretized RTE. The BiCGStab(2)/MUCS method proved to be very efficient when coupling with the
DOM/FV discretization. An efficient tabulation technique for the gaseous radiative property model SNB-FSCK using 7-point Gauss-Labatto quadrature scheme is also introduced. The proposed methodology was implemented into a highly massive parallel unstructured code. The radiation solution benefits fully from the optimized parallelism based on the dual mesh splitting.

The method was applied to calculate the radiation in a 3D rectangular enclosure containing non-isothermal homogeneous and inhomogeneous mixtures of CO₂ and H₂O. The result was reported for the heat flux and radiation energy source and comparison was also made between the present method BiCGStab(2)/MUCS/tabulated SNB-FSCK and the benchmark method SNB-CK and some other methods presented in Liu et al. [2]. The present method BiCGStab(2)/MUCS/tabulated SNB-FSCK gives more accurate predictions particularly for the radiation source term. When comparing with the benchmark solution, the relative error of the radiation source term is remarkably reduced to less than 4% as compared to 14%-18% resulted from the SNB-FSCK/M2 method in [2]. The CPU time is notably reduced and proportional to the reduction number of the narrow bands and lower than the current methods available in [2], indicating the accuracy and efficiency of the present method. The developed radiative solver was also tested with success on massively parallel platforms. Based on these advantages of the present methodology that was implemented into the proven massively parallel software YALES2, it opens an interesting way to simulate large-scale combustion systems. A future work will be dedicated to a coupling between combustion and radiation using this software.

5. References
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