A probabilistic framework for high-speed flow simulations

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1. Motivation and objectives

The thermal loads on vehicles flying at hypersonic speeds pose strict constraints on the aerodynamic design and the choice of materials. The development of computational tools that can faithfully reproduce high-Mach number flight conditions is fundamental to improve our ability to realize such vehicles especially because physical prototyping is challenging and extremely expensive. A special consideration in the development of hypersonic vehicles is the accurate evaluation of the safety and operability margins associated to specific design solutions, because of the relatively small experience with sustained hypersonic flight.

Although computational fluid dynamics (CFD) has become a common tool in the aerospace community, the use of CFD in the determination of operability limits is still in its infancy. One of the few examples is the work by Bose & Wright (2006); they have developed an approach to combine hypersonic flow solutions and a Monte Carlo sampling technique to investigate the probability to exceed critical heat fluxes at the stagnation point of capsules entering the Martian atmosphere. The environment and the physical/chemical processes at the thermal protection system are the dominant sources of uncertainties. Our objective is to develop an alternative approach adopting a novel approach, namely stochastic collocation to considerably increase the computational efficiency of evaluating reliability and safety.

One of the bottlenecks in determining the likelihood of rare events associated to failure and off-design conditions is the difficulty of assessing the true predictive capability of current computational methods. In spite of past efforts in developing accurate physical models that represent the dominant phenomena in fluid flows around high-Mach number vehicles, the confidence in numerical predictions remains limited. An additional concern is associated with the uncertainties pertaining to the differences between the designed system and the actual vehicle; these uncertainties are associated to the flight conditions, for example the stochastic changes in the atmospheric properties, the geometrical tolerances related to the manufacturing, and so forth.

With the objective of developing a computational infrastructure to perform detailed investigations of high-speed vehicles, a probabilistic framework is defined to efficiently investigate the effects of uncertainties. In the following, we refer to deterministic simulations as the computations performed by precisely defining all the input parameters such as boundary condition, phenomenological model coefficients, etc. On the other hand, probabilistic (or stochastic) computations involve random input variables: quantities defined with respect to a probability measure. The Mach number, for example, is considered to be not precisely known and defined in a range of probable values and treated as a random quantity. It is useful to point out, that in the present context, the governing equations completed with the appropriate phenomenological models are not stochastic; the randomness is artificially introduced to represent the uncertainties in either the boundary
and initial conditions, or the lack of knowledge in the physical models. Once the input parameters are defined in terms of random variables, the simulations have to be carried out by propagating the uncertainties to the output of interest. This step can be done in a straightforward way by using the Monte Carlo method; random samples are drawn from the input probability distributions and corresponding deterministic simulations are carried out. The statistics of the outputs are then computed by simple averaging. The problem with this approach is that CFD computations of realistic hypersonic vehicles require considerable computational resources, especially when 3-D and unsteady effects are considered. In addition, to quantify operability limits — in other words events with rare occurrence — the number of deterministic evaluations required in a Monte Carlo methods is very large and far beyond current computational capabilities.

A viable alternative is the use of reduced-order-models or surrogate response Robinson (2008); in this context, few deterministic simulations are carried out to build an interpolant that approximates the solutions in the parameter range of interest. The Monte Carlo approach is then applied by repeatedly sampling from this interpolant, thus not requiring additional full CFD solutions. In the present framework we employ the stochastic collocation approach of Xiu & Hesthaven (2005), were a polynomial interpolant of the output response is built.

In the following we first introduce the deterministic solver developed to perform simulation of unsteady, viscous 3-D flows in complex geometries and then describe the probabilistic framework. Examples include Sod’s shock tube problem with uncertain gas properties and the hypersonic laminar flow around a circular cylinder with uncertain viscosity.

2. Deterministic solver

A parallel solver for the solution of the compressible Navier-Stokes equations on unstructured meshes has been developed. The governing equations are written in a conservative form as:

\[ \frac{\partial}{\partial t} \int_{\Omega} U d\Omega + \int_{\partial \Omega} \left[ F(U) - F_v(U) \right] dA = 0 , \]

where \( U = [\rho, \rho \mathbf{v}, E]^T \) is the state variable, \( F(U) \) and \( F_v(U) \) are the convective and viscous fluxes, respectively, and \( \Omega \) and \( \partial \Omega \) are the physical domain of interest and its boundary.

In particular, we consider:

\[
\begin{align*}
F(U) &= [n \cdot \rho \mathbf{v}, \mathbf{v} \cdot (n \cdot \rho \mathbf{v}) + p n, (E + p)(v \cdot n)]^T \\
F(U)_v &= [0, n \cdot \Pi, v \cdot (n \cdot \Pi) + n \cdot \mathbf{Q}]^T ,
\end{align*}
\]

where \( \rho, \mathbf{v}, p, E, \Pi, \mathbf{Q}, n \) represent density, Cartesian velocity vector, pressure, total energy, stress tensor, heat flux vector and outward pointing unit vector normal to the surface, respectively. The discretization scheme is based on a finite volume formulation and implicit time-integration on arbitrary polyhedral mesh elements. The code is entirely written in C++ and uses subdomain decomposition and MPI as the parallel infrastructure.

The flow quantities are stored in the cell centers and the governing equations are integrated in conservative form:

\[ \frac{\partial U}{\partial t} = -\frac{1}{V} \sum_f [F(U) - F_v(U)] A_f . \]
2.1. Convective fluxes

In the past three decades, many different approaches have been introduced to evaluate the convective fluxes; Druguet et al. (2005) provides a comprehensive comparison of various methods. In the present solver we investigated the Roe (1981), the HLLC and the HLLE (Toro 1999) scheme.

The inviscid flux in 1-D can be linearized as

$$ F(U) = A(U) U_x. $$

The Jacobian $A(U)$ was replaced by Roe with a constant matrix $\tilde{A} = \tilde{A}(U^L, U^R)$, where $U^L$ and $U^R$ are the flow states at the two sides of a cell face. This results in a linear system with constant coefficients that retains the initial states of the exact Riemann problem. The derivation of $\tilde{A}$ is carried out enforcing several constraints: real eigenvalues (hyperbolicity), consistency with the original Jacobian and conservation of fluid properties across the shock; the details are not reported here but can be found in several textbooks, e.g., Toro (1999).

Due to the linearization of the system the resulting discretization is not positively preserving (Einfeldt et al. 1991): density and pressure can become negative within the Riemann problem evolution. Although this inconsistency is severe only in near-vacuum conditions, or when strong shocks occur, positivity might also be important in simulations where initial transients may lead to low values of pressure or density.

Furthermore, approximate Riemann solvers obtain all wavespeeds (eigenvalues of the Jacobian matrix) from an arithmetic or a square-root average of the left and right states (as for the Roe scheme). This procedure leads to an under-estimation of the expansion-wave velocity, the so-called expansion shock. Another important limitation of these schemes is the so-called carbuncle phenomenon observed, for example, at the stagnation region of blunt bodies in hypersonic flows. The convective velocity is relatively small compared to the sound speed and errors are trapped and deteriorate the solution accuracy Candler et al. (2007); Quirk (1994).

Different solutions have been proposed in the literature and can be separated in to two families: eigenvalue limiting methods and hybrid approaches.

The simple 1-D entropy fix of van Leer et al. (1989) or its multi-dimensional extension of Sanders et al. (1998) introduce artificial dissipation and limit the appearance of expansion shocks and are classified as eigenvalue limiting schemes. These modifications do not completely eliminate the occurrence of carbuncles. In addition, the multi-dimensional formulation is not easily applicable to an unstructured, parallel flow solver because it requires operations on the eigenvalues of $\tilde{A}$ corresponding to all the faces of the neighboring cells.

The second class of techniques is based on the combination of the two different approximate Riemann solvers that are blended according to the flow features to be captured (Nompelis et al. 2005; Nishikawa & Kitamura 2008).

In the present context, the Roe solver with the van Leer eigenvalue limiter is used and can be written as:

$$ |\tilde{\lambda}| = \begin{cases} |	ilde{\lambda}(\tilde{U})| & \text{if } |	ilde{\lambda}(\tilde{U})| \geq 2\eta \\ |\tilde{\lambda}(\tilde{U})|^2/4\eta + \eta & \text{if } |	ilde{\lambda}(\tilde{U})| < 2\eta \end{cases}, $$

(2.5)

where $\eta$ is a function of the left and right states $\eta = \max(\lambda^R - \lambda^L)$. As previously mentioned, the original van Leer limiter does not entirely eliminate the
occurrence of carbuncles, because $\eta$, which controls the amount of dissipation can vanish in stagnation regions.

The second approximate Riemann solver implemented in the present context is the HLLC scheme proposed by Toro et al. (1994) and Batten et al. (1997). In this method the entropy condition is enforced (no entropy violating discontinuous waves, called rarefaction shocks) and the scheme preserves positivity without the need for additional corrections.

The convective flux is evaluated as:

$$F^{HLLC} = \begin{cases} 
F(U_l) & \text{if } S_L > 0 \\
F(U_l) + S_L(U^*_l - U_l) & \text{if } S_L \leq 0 < S_M \\
F(U_r) + S_R(U^*_r - U_r) & \text{if } S_M \leq 0 \leq S_R \\
F(U_r) & \text{if } S_R < 0 
\end{cases} \tag{2.6}$$

The wavespeeds $S_L$ and $S_R$ correspond to the left and the right acoustic waves, whereas $S_M$ is related to the intermediate contact/shear characteristic. If the flow is supersonic from left to right the acoustic wavespeed is $S_L > 0.0$ and the flux has contribution from the left state only; conversely the flux is evaluated from the right state in the case of $S_R < 0.0$. In subsonic conditions the flux evaluation is further subdivided to ensure accuracy at the contact surfaces, where $U^*_l$ and $U^*_r$ are the corresponding states. A detailed description of the scheme can be found in Batten et al. (1997).

The third investigated approximate Riemann solver is HLLE (Einfeldt et al. 1991) and can be seen as a reduced order scheme of HLLC in which the intermediate stage between the left and right sound waves is approximated by one stage only. This scheme does not exactly resolve isolated contact discontinuities. As a contact discontinuity is numerically equivalent to a limiting case of a viscous boundary layer the disadvantage of this scheme is the dissipative property close to walls.

Figure 1 shows the result of an inviscid computation for the 2-D flow around a cylinder flow at Mach 5.0 on a grid consisting of 200 x 60 cells in the circumferential and radial direction, respectively. The Roe scheme with the van Leer limiter produces the carbuncle in the front stagnation region as expected. By using a fixed high value of $\eta = 3.0$ in Eq. (2.5) this spurious feature can be eliminated, but high artificial dissipation is now present across the shock and in the entire flowfield. This can substantially degrade the accuracy of viscous simulation. Hybrid methods use the eigenvalue limiter only outside
viscous layers (see Gnoffo & White 2004) but have not been investigated here. The results obtained with the HLLC scheme are more encouraging although far from perfect as the symmetry along the stagnation streamline is altered. Further work is currently ongoing to improve the accuracy of the convective flux evaluation. A possible solution could be a hybrid methodology by using the HLLE scheme (gives a symmetric solution for the inviscid cylinder flow) in restricted areas and a more accurate scheme elsewhere Quirk (1994).

2.2. Higher order reconstruction and slope limiting

The convective flux evaluation illustrated in the previous section leads to a first-order accurate scheme. High order accuracy is typically achieved by computing the states at each side of a given cell face using high-order interpolation and then applying the same flux evaluation scheme to the reconstructed states. On an unstructured grid the reconstruction is formulated as

$$\phi_L^f = \phi_P + \psi_P \nabla \phi|_P \cdot r_f,$$

(2.7)

where $\nabla \phi$ is a discrete approximation of the gradient at $P$, computed using standard least squares approximation or the Gauss theorem. Across a discontinuity and, in general, in regions where the solution is changing rapidly a slope limiter is used to modify the second term in Eq. (2.7); for a review of slope limiters as well as issues that can arise on unstructured grids, see Berger et al. (2005).

In the present work, we explored an alternative approach to slope limiting which is based on a solution-weighted least squares gradient (SWLSG) approximation. Mandal & Subramanian (2008) have shown that this approach with judicious choice of weights does not require the application of limiters; Mandal & Subramanian (2008) have used this approach to solve the inviscid Burger equation and a 2-D linear convection problem.

In the present context the SWLSG is formulated as

$$\phi_L^f = \phi_P + \nabla \phi|_P \cdot r_f,$$

(2.8)

with the weighted least squares gradient $\nabla \phi$ in which the weights depend on $\phi$. For the
sake of clarity we write the gradient construction for 1-D with uniform spacing between
the cell centers
\[ \frac{\partial \phi}{\partial x} \bigg|_P = \frac{w_w \delta \phi_w + w_e \delta \phi_e}{(w_w + w_e) \Delta x}, \tag{2.9} \]
where the indices \( w \) and \( e \) denote the west and east side of the cell \( P \). It can be mathematically shown that by taking the weights
\[ w_w = \frac{1}{(\delta \phi_w)^2} \quad \text{and} \quad w_e = \frac{1}{(\delta \phi_e)^2}, \tag{2.10} \]
the gradient reconstruction in Eq. (2.8) recovers the common slope limiter of van Al-
bada et al. (1982). Further Mandal & Subramanian (2008) show how, with only minor
modifications, many of the common slope limiters can be expressed as weighted least
squares approaches. Due to the symmetric form of Eq. (2.9) (weights are evaluated the
same on each face), the construction for multiple dimensions and unstructured grids can
be obtained like commonly used least squares approaches.

Figure 2 shows the results obtained using the SDWLS scheme, a first-order solution
and a conventional van Albada slope limited approach. The problem is the classic 1-
D Sod’s shock tube and the computations are performed with the HLLC approximate
Riemann solver on a uniform grid with 400 control volumes. As expected, the SDWLS
approach reproduces exactly the van Albada solution and is accurate in reproducing this
flow solution. As an additional test of the present unstructured grid formulation, we
performed computations on a coarse 2-D unstructured mesh with a highly irregular grid
pattern in the center of the domain. The computational results reported in Fig. 3 show

Figure 3. The SDWLS approach for Sod’s shock tube on a unstructured grid.
all the grid cells in the domain – we expect the solution to remain 1-D. Despite a small spreading in the region of strong grid non-uniformity \((x = 1)\) the solution is reproduced accurately and the speed of the characteristics is consistent with the analytical solution.

2.3. Viscous fluxes

The viscous fluxes contain second derivatives of the velocity \(u\) and the temperature \(T\). Therefore, gradients at the cell face need to be calculated in an efficient and accurate way. Consider the scalar quantity \(\phi\), whose gradient at the cell face is \(\nabla \phi\). We approximate the normal gradient at the face as

\[
\nabla \phi|_f \cdot n_f = \frac{\phi_{nbr} - \phi_P}{|x_{nbr} - x_P|} \alpha_f + \frac{1}{2} (\nabla \phi|_P + \nabla \phi|_{nbr}) \cdot (n_f - \alpha_f s_f),
\]

where the subscript \(f\) indicates the face with the adjacent control volumes \(P\) and its neighbor \(nbr\) (Ham & Iaccarino 2004). The vector \(n\) is the face normal and \(s\) is the normalized vector connecting the cell centroid across the face \(f\). The gradients \(\nabla \phi\) at the cell centers are computed using a least squares approximation. The tangential velocity gradients are also evaluated in the same way. Note that for the viscous fluxes the SWLSG approach is not used.

Figure 4 shows a 2-D laminar flow around a cylinder at \(Ma = 5.7\) with a Reynolds number of 16500. The qualitative comparison between computation and experiment shows overall agreement with a satisfactory correspondence of the main flow structures: the strong bow shock in front of the cylinder, the horizontal shocks above and below the cylinder separation region and the oblique trailing-edge shocks.

2.4. Time integration treatments and scalability

The governing equations form a non-linear system that is typically solved using an explicit time-integration scheme or a Newton procedure with implicit inner iterations. Three different time-integration schemes are currently being evaluated:
R. Pečnik et al.

- explicit third-order Runge-Kutta (RK) scheme;
- fully coupled implicit scheme based on a bi-conjugate gradient (BCGStab) solver, Barrett et al. (1994);
- Gauss-Seidel point (PGS) relaxation scheme.

Taylor expansion is used to formulate the implicit schemes for the inviscid and viscous fluxes:

$$F^{n+1} \approx F^n + \left. \frac{\partial F}{\partial U} \right|_n \delta U + O(\delta U)^2. \quad (2.12)$$

The Jacobian of the Roe flux scheme is very simple and is not reported here; the implicit form of the HLLC scheme is based on the wavespeeds decomposition reported in Eq. (2.6):

$$F^{n+1}_{HLLC} = \begin{cases} 
F^n_l + \frac{\partial F_l}{\partial U} \delta U_l \\
F^n_l + S^n_L (U^n_l - U^n_r) + \left[ \frac{\partial F_l}{\partial U} + S^n_L \left( \frac{\partial U_l}{\partial U} - I \right) \right] \delta U_l + S^n_L \frac{\partial U_l}{\partial U} \delta U_l \\
F^n_r + S^n_R (U^n_r - U^n_l) + \left[ \frac{\partial F_r}{\partial U} + S^n_R \left( \frac{\partial U_r}{\partial U} - I \right) \right] \delta U_r + S^n_R \frac{\partial U_r}{\partial U} \delta U_r \\
F^n_r + \frac{\partial F_v}{\partial U} \delta U_r
\end{cases} \quad (2.13)$$

with the Jacobean matrix $\frac{\partial F}{\partial U}$ and the matrix $\frac{\partial U^*}{\partial U}$, which is discussed in Batten et al. (1997).

The viscous flux is linearized as

$$F^{n+1}_v = F^n_v + \frac{\partial F_v}{\partial U} \delta U_l + \frac{\partial F_v}{\partial U} \delta U_r \quad (2.14)$$

with

$$\frac{\partial F_v}{\partial U} = A_v = \frac{\partial F_v}{\partial Q} \frac{\partial Q}{\partial U} \quad (2.15)$$

and with $Q = [u \ v \ w \ T]^T$ and $\partial Q/\partial U$ based on Pulliam & Steger (1982).

The inviscid flow around a cylinder at $Ma=5$ is used to compare the three approaches (see Fig. 1); the convective fluxes are evaluated using the HLLC approximate Riemann solver without high-order reconstruction. The time steps required to achieve convergence to steady state (and the associated computational cost) are reported in Fig. 5.

The use of high-order reconstructions and non-continuous limiter functions can often stall the convergence to steady state. One possible solution is to use more diffusive limiters; another alternative is to modify the time-integration scheme (Batten et al. 1997) by the use of two successive backward Euler steps as follows:

$$\delta U = \text{solve lin. system} \left( U^n, \Delta t/2 \right)$$
$$U^{n+1/2} = U^n + \delta U$$
$$\delta U = \text{solve lin. system} \left( U^{n+1/2}, \Delta t \right)$$
$$U^{n+1} = U^{n+1/2} + \delta U/2. \quad (2.16)$$

In Fig. 6 comparisons between the conventional backward Euler scheme and the modified one are reported for the calculation of the cylinder flow with the HLLC scheme, the SWLSG approach and the PGS relaxation.
Figure 5. Inviscid Mach 5.0 cylinder flow. Solution residual using Runge-Kutta, Point Gauss-Seidel and fully implicit BiCGSTAB time integration solvers.

Figure 6. Solution residual for second-order computations using different time-integration schemes.

3. Stochastic solver

The determination of the effect of uncertainties on numerical predictions is based, in this work, on a probabilistic framework. The first step consists in the definition of the uncertainty sources; these are then described by a set – potentially very large – of random variables with an associated joint probability distribution. Afterward the uncertainty is propagated through the computational model and the resulting uncertainty in the output quantities of interest is quantified by computing their statistics, such as expectation, variance and probability density functions. The propagation techniques can be classified into two categories: (1) non-intrusive, where existing deterministic solvers can be used as black box function evaluations, and (2) intrusive, where existing solvers must be modified to account for introduction of uncertainty into the model. The focus on this work is on non-intrusive techniques, combined with the deterministic solver described previously.

The goal with non-intrusive techniques is to achieve the highest accuracy with the least
number of function evaluations to limit the overall computational overhead associated to the uncertainty analysis.

Assume the randomness in the model can be characterized by a finite set of \( d \) independent random variables denoted \( Y = \{Y_1, \ldots, Y_d\} \). In the examples included here \( Y \) describes the uncertainty (precisely the stochastic variability) of physical quantities specified as boundary conditions or the material properties of the fluid. The overall objective is to compute the stochastic solution \( U(x, t, Y_1, \ldots, Y_d) = U(x, t, Y) \). Stochastic collocation achieves this goal by computing statistics such as expectation, variance and probability density functions. The full stochastic problem is reduced to a set of uncoupled deterministic problems: for \( k = 1, \ldots, K \) choose \( Y^{(k)} \) from the range of variability of \( Y \); then solve \( K \) deterministic problems of the form

\[
\frac{\partial}{\partial t} \int_{\Omega} U(x, t, Y^{(k)}) \, d\Omega + \int_{\partial\Omega} \left[ F \left( U(x, t, Y^{(k)}) \right) - F_v \left( U(x, t, Y^{(k)}) \right) \right] \, dA = 0. \tag{3.1}
\]

The computed solutions \( U(x, t, Y^{(k)}) = U^{(k)} \) corresponding to \( Y^{(k)} \) are used to compute statistics of the stochastic solution.

The main ideas behind stochastic collocation are multi-dimensional interpolation and integration rules in the probability space: the space induced by the random parameters \( Y \). In theory, any spatial discretization technique can be used to characterize the behavior of the solution as the values of \( Y \) change. With interpolation, we construct a response function of \( Y \) that approximates the actual solution, and this approximation is exact at the collocation points, \( Y^{(k)} \). We then integrate along the coordinates of \( Y \) to compute statistics such as expectation and variance (Ganapathysubramanian & Zabaras 2007; Nobile et al. 2007; Xiu & Hesthaven 2005).

### 3.1. Interpolation

In one dimension, it is easy to construct a Lagrange-polynomial-based interpolant of a function \( f(y) \) defined on \([-1, 1]\) (note that the extension to a bounded domain \([a, b]\) is trivial). Choose a sequence of \( K \)-point abscissas \( \{y_1, \ldots, y_K\} \subset [-1, 1] \). The interpolant is a linear combination of Lagrange polynomials weighted by the function \( f \) evaluated at the points in the abscissa. Specifically, we define an interpolation operator \( \mathcal{U} \) as

\[
\mathcal{U}(f(y)) = \sum_{j=1}^{K} f(y_j) \ell_j(y),
\]

where \( \ell_j(y) = \prod_{k=1, k\neq j}^{K} \frac{y - y_k}{y_j - y_k} \) is the Lagrange polynomial of degree \( K - 1 \). The interpolant \( \mathcal{U} \) is unique and equals \( f(y) \) at each point in the abscissa. With a properly chosen abscissa and some mild conditions on \( f \), the interpolant will converge exponentially pointwise to the actual function as the number of points \( K \) goes to infinity.

The natural extension of interpolation to multiple dimensions is a tensor product of 1-D interpolants. Now let \( F(y_1, \ldots, y_d) \) be defined on the hypercube \( \Gamma = [-1, 1]^d \), where \( d \) is the number of dimensions. Following standard notation, we introduce a multi-index \( i = (i_1, \ldots, i_d) \). The abscissa for the multi-dimensional interpolant is simply the tensor product of the abscissas for the 1-D interpolants:

\[
\{y_1^{i_1}, \ldots, y_K^{i_1}\} \times \cdots \times \{y_1^{i_d}, \ldots, y_K^{i_d}\}.
\]

Note that the number of points in the abscissa is \((mK)^d\), which increases exponentially as \( d \) increases. It is possible to generalize the construction to allow a different number of
A probabilistic framework for high-speed flow simulations

abscissas in each direction $d$. We construct the full tensor product interpolant as

$$I_i = (U^1 \otimes \cdots \otimes U^d)(f) = \sum_{j_1=1}^{K} \cdots \sum_{j_d=1}^{K} F(y_{j_1}, \ldots, y_{j_d})(\ell_{j_1} \otimes \cdots \otimes \ell_{j_d}).$$

The computational cost associated to tensor grid extension of 1-D quadrature rule limits the applicability of this approach to a moderate number of dimensions, e.g., $d \leq 5$. The sparse grid formulation originally described by Smolyak (1963) offers a more economical strategy for dealing with problems with a large number of uncertain variables. The sparse grid collocation approach has been implemented but is not reported here for brevity.

3.2. Integration

Once we construct an interpolant of $F$, approximating an integral of $F$ reduces to computing integrals of the basis polynomials. For example,

$$\int_{\Gamma} F \, dy \approx \sum_{j_1=1}^{K} \cdots \sum_{j_d=1}^{K} F(y_{j_1}, \ldots, y_{j_d}) \left( \int_{\Gamma} \ell_{j_1} \otimes \cdots \otimes \ell_{j_d} \, dy \right) = \sum_{j_1=1}^{K} \cdots \sum_{j_d=1}^{K} F(y_{j_1}, \ldots, y_{j_d}) w(j_1, \ldots, j_d),$$

where $w(j_1, \ldots, j_d)$ is the weight associated with the $d$-dimensional abscissa $(y_{j_1}, \ldots, y_{j_d})$. This formula can be interpreted as a familiar multi-dimensional cubature rule.

3.3. Choice of abscissa

Each of the specific interpolation formulas and integration rules depends on the choice of abscissa. The predominant choices in the literature are the Clenshaw-Curtis and Gaussian abscissas. Both of these choices have attractive properties.

The Clenshaw-Curtis abscissas are the extrema of the Chebyshev polynomials in the interval $[-1, 1]$. For any choice of $K > 1$, these points are given by

$$y_j = -\cos \left( \frac{\pi (j - 1)}{K - 1} \right), \quad j = 1, \ldots, K.$$ 

This quadrature rule has the interesting property that with the proper choice of successive quadrature levels $K_1$ and $K_2 > K_1$, the corresponding abscissas are nested sets, which means that to achieve the next level of accuracy, one can use the function evaluations from the current level and need not recompute all function values from scratch. Also, in practice, this makes convergence easy to check. Once one has evaluated the function at all points necessary for computing statistics at level $K$, the statistics can be quickly computed for all levels up to and including $K$ to observe convergence.

The proper choice of the sequence $K_i$ that induces this cost-saving nested property is

$$K_1 = 1 \quad \text{and} \quad K_i = 2^{i-1} + 1, \quad \text{for } i > 1.$$ 

This choice doubles the number of points on either side of zero (the midpoint) at each successive increment of $i$. Choosing $K_1 = 1$ is crucial to keeping the number of points in the sparse grid manageable as $d$ increases.

For integration, it is very useful to precompute the weights; the following closed formula
are used for 1-D integration:
\[
w_j = w_{K+1-j} = \frac{2}{K-1} \left( 1 - \frac{\cos(\pi(j - 1))}{K(K - 2)} \right) - 2 \sum_{k=1}^{(K-3)/2} \frac{1}{4k^2 - 1} \cos \left( \frac{2\pi k(j - 1)}{K - 1} \right)
\]
for \( j = 2, \ldots, K - 1 \) with the two missing weights
\[
w_1 = w_K = \frac{1}{K(K - 2)}.
\]
The \( K \)-point Clenshaw-Curtis quadrature rule can exactly integrate any polynomial of degree \( K - 1 \), and its accuracy is often stated in these terms. There is a sizeable body of literature on the properties and error analysis of the Clenshaw-Curtis quadrature rules, for example, Trefethen (2007) and its references.

The Gaussian abscissas are the zeros of the polynomials that are orthogonal with respect to a positive weight function. In practice, the weight function should be the probability density function \( \rho \) of the parameterizing random variables. For example, in the case presented in the following, parameters are independent random variables distributed uniformly over \([-1, 1]\), so that \( \rho = (1/2)^3 \). The orthogonal polynomials associated with this weight function are tensor products of Legendre polynomials defined on \([-1, 1]\). Therefore the Gaussian abscissas are the zeros of the Legendre polynomials. In general these point sets are not nested; however, there are extensions to Gaussian rules that are nested (see Kronrod 1965).

In terms of accuracy of integration, the Gaussian rules are known to be the most accurate, theoretically. A \( K \)-point Gaussian rule will exactly integrate a polynomial of degree \( 2K - 1 \). For additional discussion on the theoretical properties of Gaussian quadrature, see Isaacson & Keller (1994).

Two application of stochastic collocation are presented below. In both cases only one uncertain parameter is considered. The first problem is Sod’s shock tube test reported before but with uncertain gas properties. In particular, the ratio of the specific heats, \( \gamma \) is chosen to be a uniform random variable, \( 1.2 < \gamma < 1.6 \).

We compare the accuracy of Gauss-based collocation point using \( K = 3 \) and \( K = 10 \) function evaluations. In addition, we used the conventional Monte Carlo method with \( K = 1000 \) samples to verify that the statistics are in agreement.

The results are reported in Fig. 7 in terms of the expectation and the standard deviation of the density. The input uncertainty (in \( \gamma \)) is not very dominant and the overall density profile within the tube is only slightly affected. A more detailed analysis of the density across the right-moving shock shows that the collocation approach indeed represents the statistics in excellent agreement with the Monte Carlo solution, although at a cost reduced by two orders of magnitude. It is also interesting to note that the solution obtained using low-order collocation \( (K = 3) \) results is in general agreement with the other solutions but illustrates the occurrence of a non-smooth density profile across the shock. This phenomena has been observed and analyzed in Pettersson et al. (2008).

The second example shows the laminar flow around the circular cylinder at \( Ma = 5.7 \) subject to uncertainty in the molecular viscosity; the corresponding variability in the Reynolds number is \( Re = 16500 \pm 10\% \). In this case, given the computational cost associated to each deterministic simulation, only the stochastic collocation approach has been used with \( K = 10 \) quadrature points. The results are shown in Fig. 8 in terms of the standard deviation of the density. The change in the Reynolds number induce an increased stand-offdistance and a misplacement of the wake shocks. Further work
4. Conclusion and future work

Numerical simulations of hypersonic flows in the presence of uncertainty require the development of a probabilistic framework; the present computational tools have been introduced and verified for the simulation of simple problems, namely the inviscid, unsteady, 1-D flow in a shock tube and the viscous flow around a cylinder. Initial uncertainty quantification simulations based on the stochastic collocation approach are also reported. Initial comparisons with Monte Carlo simulations show computational saving of two orders of magnitude, albeit for problems involving only one uncertain parameter. Current work is focused on multi-dimensional extension, in particular based on the sparse grid formalism.

In addition, the deterministic solver is currently being extended to include the effect of turbulence using Reynolds averaging modeling.
Figure 8. Standard deviation of density for the viscous $Ma = 5.7$ cylinder flow; Reynolds number: uniform random $Re = 16500 \pm 10\%$; stochastic collocation with 10 quadrature points; approximate Riemann solver: HLLE.

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