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Locally-Adaptive Tabulation of Low-Dimensional Manifolds using Bézier Patch Reconstruction

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Abstract

An efficient tabulation strategy for turbulent combustion simulations is proposed. Using a locally adaptive arrangement of structured Bézier patches–often used in computer graphics–the combustion manifold can be efficiently tabulated; thus reducing the table size by over an order of magnitude while maintaining high accuracy. A hybrid search algorithm is implemented that uses a one-step quadrant analysis followed by a linear search to minimize the cost of the data retrieval. The present tabulation has been successfully applied to flamelet/progress variable approach (FPVA) and trajectory generated low-dimensional manifold (TGLDM). The error, computational size and search-and-retrieval time are quantified and compared against classical tabulation approaches.

1 Introduction

The accurate computation of the detailed chemical kinetics is essential to capture the full-complexity of the physical processes involved in many turbulent combustion simulations. Despite the drastic increase in computational power, it is still unrealistic to account for the hundreds to species and thousands of different reactions that are needed in modern hydrocarbon mechanisms [1]. The multi-dimensionality renders the problem intractable and mechanism reduction is inevitable. One reductive approach consists of defining a skeletal or reduced mechanism to limit the total number of species under consideration, thus eliminating tertiary species and reactions pathways. The remaining chemical reactions and species must nonetheless be integrated in time. A more efficient approach consists of taking advantage of the spatial or temporal scale separation in order to reduce the dimensionality of the problem by bounding the degrees of freedom. In some specific regimes, the scale separation can further be used to justify a pre-tabulation in order to offer an even greater reduction in computational cost. By pre-computing and tabulating the chemistry, the expensive run-time differential equation integrations can be replaced by an efficient table-lookup.

The advantages of dimension reduction combined with *a priori* tabulation are well accepted and used in a number of reactive flow simulations. In a flamelet regime, the local non-premixed flame structure can be represented as a laminar diffusion flame; a trivial run-time look-up provides the needed source terms and composition to the governing equations. Similarly, in conditional source-term estimation (CSE) or conditional moment closure (CMC), a pre-tabulation of the trajectory generated low-dimensional manifold (TGLDM) is done using a perfectly-stirred, 0-D reactor in order to accurately map out the compositional state of the reaction processes. Other tabulation strategies are found in the literature. Pope proposed the *in situ* adaptive tabulation (ISAT) [2] that tabulates, during run-time, and stores the information in a binary tree. Ihme *et al.* [3, 4] developed an optimal artificial neural network (OANN) which showed a dramatic decrease in the memory footprint (about 5000 times smaller table size for a similar level of accuracy) but proved to be about 3 times slower than a conventional, homogeneous tabulation strategy. A combination of ISAT and OANN has also been proposed [5]. Other approaches, such as PRISM, rely on polynomial regressions to define the surface of a hypercube [6]; the main drawback in the computational expense of the high-dimensional tables. Adaptive chemistry models based on the Computational Singular Perturbation-slow-manifold projector show a very good accuracy and reliability but comes at a computational cost [7].

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In many of these approaches, the way in which the information is stored remains primitive. Typically, the Flamelet Progress-Variable Approach (FPVA) [8, 9] relies on a structured tabulation. An equidistant grid is used to map the flamelets in mixture fraction ($\widetilde{Z}$) and progress variable ($\widetilde{C}$) space; a non-homogeneous discretization is used for the variance of the mixture fraction ($\widetilde{Z''^2}$). On the other hand, TGLDM often uses a Delaunay triangulation to tabulate the compositional states [10] as a function of four dimensions [11]: mass fraction of two species (CO_2 and H_2O), enthalpy and mixture fraction. Considering the sizable effort invested into the construction of these models, surprisingly little effort has been placed on the actual tabulation itself. These classic approaches quickly become intractable when additional physics (*e.g.* pressure variation, radiative heat transfer effects, partial premixing, multi-fuel) or a higher-dimensional manifold is considered. The increased dimensionality results in either: (i) a reduction in the table resolution; or (ii) an increase in computational table size. Both have significant consequences on the accuracy and computational efficiency of the simulation. One should keep in mind that pre-computed tables have an insidious effect on computational time. As each processor must directly access the tabulated values, an increased table size imposes severe limitations on the available random access memory (RAM) and may impact the data locality in the various levels of the cache. Therefore, the increased dimensionality quickly renders tabulation ineffective.

Based on these observations, a novel approach is proposed to drastically reduce the memory footprint of FPVA and TGLDM tabulations. This work only seeks to improve how we tabulate the data, not what we tabulate. Taking inspiration from computer graphics, we use a locally-adaptive structured mesh as a support for Bézier patches to describe the chemistry. By controlling the local adaptation of the structured mesh, the complex chemistry data can be fitted to a user-defined error tolerance. The approach, based on the developments of Collins and Luke [12] for the representation of multi-phase state diagrams, allows an order of magnitude table size reduction while slightly affecting the computational look-up time.

The remainder of the paper is organized as follows. The theoretical background of the recursive Bézier table construction is presented in the following section. The algorithm is then applied to the discretization of FPVA and a TGLDM tables; the error evaluation, memory reduction and look-up time are carefully evaluated in §3. Finally, in §4, the results are discussed and further improvements to the model are proposed.

2 Recursive Bézier patch reconstruction

A tabulation strategy is proposed based on a recursive Bézier patch reconstruction. The tabulated values are represented by a structured arrangement of Bézier patches which are defined using third-degree Bernstein polynomials, see Equation (1). The corners of the patches are determined by a recursive refinement strategy, which allows a local clustering to optimize the total number patches needed to represent the desired topology. The refinement strategy follows a quad-tree approach, where each patch that does not fall within the user-defined tolerance is sub-divided into four patches and re-evaluated. The control points and boundaries of each patch are pre-tabulated.

A Bézier patch is defined mathematically over an arbitrary orthonormal coordinate system as:

$$F(u,v) = \sum_{i=0}^{3}\sum_{j=0}^{3} B_i^3(u) B_j^3(v) b_{ij} \qquad \text{where} \qquad B_i^3(u) = \frac{3!}{i!(3-i)!}\,(1-u)^{3-i}\,u^i \tag{1}$$

where $B_i^3(u)$ are the third-degree Bernstein polynomials and $b_{i,j}$ are the 16 control points. The Bernstein polynomials can be evaluated at the parametric locations $u \in [0,1]$ and $v \in [0,1]$ to obtain the blending coefficients. The patch fitting follows the algorithm outlined in [12]. Let $B_{i,j} = B_i^3(u)B_j^3(v)$, $\mathbf{B}$ be the 16×16 matrix of calculated $B_{i,j}$, $\mathbf{f}$ be the vector of 16 sampled values and $\mathbf{b}$ be the vector of 16 control points. With 16 equations and 16 unknowns, the system of equations can be expressed as: $\mathbf{f} = \mathbf{B}\mathbf{b}$. The control points can be found by inverting the matrix: $\mathbf{b} = \mathbf{B^{-1}}\mathbf{f}$. These control points are tabulated for each patch and are used to evaluate any points within the patch. Solving for the control points in this way guarantees that the patch will intersect the 16 sampled values.

The refinement strategy begins by dividing the entire domain into four quadrants. Since the matrix equation requires 16 sampled values per patch, each patch is calculated by sampling points that are equally spaced in either direction within the patch range, corresponding to the locations for $m, n = \{0, 1, 2, 3\}$, where $u = \frac{m}{3}$ and $v = \frac{n}{3}$. After the control points are calculated, the error is evaluated. A number of points are taken from the

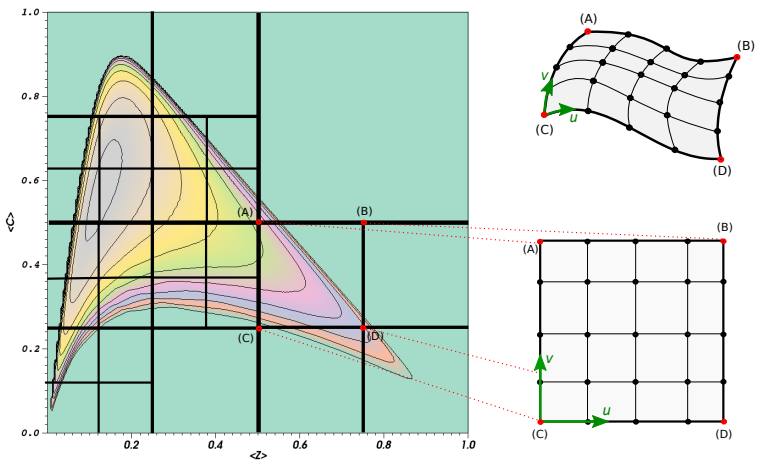

Fig. 1: Illustration of the local grid adaptation and Bézier patch with support points.

data and recalculated using the Bézier surface at the same locations. In our case, the maximum grid size for error evaluation was 200x200 and the minimum was 4x4, which is a guaranteed fit. The error is quantified by computing and comparing the double numerical integral of each. If the error of the patch is not within the specified tolerance, the patch is then divided into four children patches to be re-evaluated. An illustration of the quad-tree approach and the coordinate system of each Bézier patch is shown in Figure 1.

2.1 Search algorithm

The patches are sorted into four quadrants during the table creation. A single-step, quad-tree search is undertaken to identify the initial quadrant of the query. The search then starts from the top-left patch of the identified quadrant and traverses the table down and then right until the desired patch is found. The hybrid quad-tree/linear approach provides a compromise between data accessibility and computational efficiency. The result is computed by mapping the global coordinates onto the parametric coordinate systems of the patch.

We solve the patch at the parametric coordinates with the control points of the identified patch. The surface is solved with the matrix equation:

$$P = \mathbf{UMbM}^{\mathrm{T}}\mathbf{V}^{\mathrm{T}} \qquad \text{where} \qquad \mathbf{M} = \begin{bmatrix} -1 & 3 & -3 & 1 \\ 3 & -6 & 3 & 0 \\ -3 & 3 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}; \qquad \mathbf{U} = \begin{bmatrix} u^3 \\ u^2 \\ u \\ 1 \end{bmatrix}^T; \qquad \mathbf{V} = \begin{bmatrix} v^3 \\ v^2 \\ v \\ 1 \end{bmatrix}^T.$$

where $\mathbf{b}$ is the 4×4 matrix of control points and $\mathbf{M}$ is the Bézier basis matrix. The rows of the basis matrix are the coefficients of the third degree Bernstein polynomials.

3 Analysis and Results

In this section, the locally-adaptive Bézier patch reconstruction is applied to a FPVA and a TGLDM tabulation. The accuracy, memory requirement, and computational cost for each approach is evaluated.

3.1 High-pressure FPVA tabulation

A set of 306 counterflow diffusion flames at transcritical conditions is simulated. The H_2/O_2 flamelets cover all realizable conditions for the given pressure (7 MPa) and temperature inlet (H_2/O_2: 195 K/120K) states. Each flamelet is composed of 1000 grid points and the mesh was adapted to cluster the points in regions with large gradients. The high-pressure H_2/O_2 combustion mechanism by Burke *et al.* [13] was used for the chemical kinetics. A Peng-Robinson state equation accounts for the complex thermodynamics while Chung's

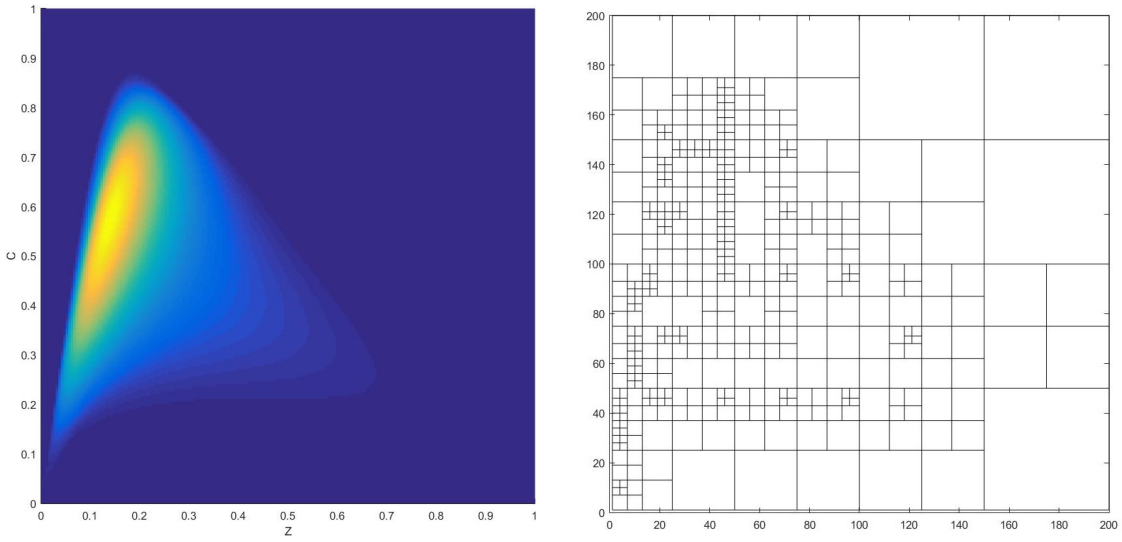

Fig. 2: Adaptive Bézier patch arrangement on the heat release term of the flamelet table. The heat release as a function of the mixture fraction and progress variable flamelets (left) and the local adaptation of the support points for the Bézier patches (right).

approximations [14] are used for the thermophysical quantities. The transcritical nature of the flamelets leads to a pseudo-phase change in the oxidizer, which results in large gradients that need to be captured in the tabulation. The transcritical flamelet represents a more challenging case compared to standard gaseous flamelets.

The standard FPVA tabulation maps the flamelets as a function of the mixture fraction, $\widetilde{Z}$, and progress variable, $\widetilde{C}$ (here defined as the mass fraction of H_2O). The grids in both dimensions are typically homogeneous to facilitate run-time data retrieval. The turbulence-chemistry interaction is obtained by convolving a presumed probability density function and extending the table in the third dimension. The resulting convolution is mapped to the standard deviation of mixture fraction, $\widetilde{Z''^2}$, typically with a logarithmically scaled grid spacing. Since the additional dimension essentially smooths out the chemistry description in $\widetilde{Z}$ and $\widetilde{C}$ space, we only consider a two-dimensional table for this study.

For a standard FPVA table, the accuracy is directly related to the number of homogeneously spaced grid points. The variation of the tabulation error with regards to the table size is a particularly important metric. To quantify the tabulation error in the classical FPVA, the flamelet set were interpolated onto homogeneous grids at various resolutions (see Table 1). A random set of 100 flamelets were then compared against the extracted values from the table. For smooth variables in mixture fraction space, such as temperature or oxidizer mass-fraction, the average maximal error (normalized with the maximum value of each flamelet) for all sampled the flamelets varies from about 16% for the coarsest table to just under 4% for the finest mesh. For variables with larger local gradients such as heat release, the average maximal error is about 10% for the finest table. The reduction in the maximum error and error root-mean-square relative to the coarsest table is shown in Table 1. Because of the strong nonlinearities in the chemistry representation, a homogeneous, structured tabulation is ineffective at drastically reducing the tabulative error.

The recursive Bézier patches were applied to the mapping of the heat release of the FPVA table (see Figure 2), the most non-linear variable in the present chemistry table. Table 1 shows that the memory usage increases linearly with the number of Bézier patches while the relative error reduces much more rapidly. By doubling the number of patches describing the chemistry, the error is reduced by about an order of magnitude. For relatively coarse tables, the memory saving is modest (about 35% size reduction); for very fine tables the size reduction is significant (about 2 orders of magnitude). Despite an increase in data complexity compared to homogeneous tables, the data retrieval time remains acceptable. The total search time for 100,000 table queries is on the order of one second. Furthermore, by doubling the number of patches, only a slight increase in the search time is noted (see Table 1).

Table 1: Comparison of standard (top) and Bézier reconstructed FPVA table at various resolutions. Total memory footprint considers a three-dimensional table with 7 stored variables. The relative error and search time is considered relative to the coarsest table.

Standard FPVA

Table size: $\widetilde{Z} \times \widetilde{C}(\times\widetilde{Z''^2})$	Size (Mb)	Relative maximum error	Relative average error rms
100×100(×13)	7.1	1	1
200×200(×25)	56.8	0.32	0.51
400×400(×50)	455	0.23	0.30
800×800(×100)	3,640	0.29	0.25
2000×2000(×200)	43,750	0.22	0.22

Bézier reconstructed FPVA

Table size: Nb patches ($\times\widetilde{Z''^2}$)	Size (Mb)	Relative error	Relative search time
469 (×13)	4.586	1	1
748 (×25)	13.79	0.2	1.05
1225 (×50)	43.75	0.01	1.07
2020 (×100)	141.4	0.00002	1.18
2206 (×200)	310.8	1e-20	1.61

Table 2: Bézier patch reconstruction of the H_2 source term of a TGLDM table.

Nb of patches (× mix. fraction)	Size (Mb)	Absolute maximum error	Search time (s)
799 (×25)	2.37	1.0e-15	0.93
1174 (×25)	3.38	5.0e-16	0.96
2938 (×25)	8.10	5.0e-17	1.00

3.2 Trajectory generated low-dimensional manifold

The use of locally-adaptive Bézier patches is applied to a trajectory generated low-dimensional manifold (TGLDM) for the combustion of pure methane and air. By defining the initial conditions on the realizable bounds, the trajectories are generated and mapped onto a space defined by the mass fraction of H_2O and CO_2. In this basis, the individual trajectories are interpolated using a Delaunay triangulation to cover the entire realizable space. In essence, the queried tabular values are linearly interpolated between the discrete set of points describing the trajectories.

The memory footprint for a triangulated table remains large. If we consider M trajectories (for a given mixture fraction) each described by a total of N points, the resulting Delaunay triangulation requires storage of $N * M$ floats (points), $N * M * (2 + 1)$ integers (simplices) and $N * M * (2 + 1)$ integers (neighbors), for each stored variable. For example, 50 trajectories each containing 50 points requires about 0.33 Mb per mixture fraction; if 25 mixture fractions are used, the total table size would be about 8.3 Mb (assuming 15 tabulated variables). Using a Bézier patch reconstruction, shown in Figure 3, the tabulated trajectories can be more efficiently stored, although the benefit is far less than for FPVA, as the memory footprint remains on the same order of magnitude at the Delaunay triangulation, as shown in Table 2. The benefits of the Bezier reconstruction lies in the more efficient data search. Similar to the FPVA table, 100,000 table queries are completed in about one second.

4 Conclusion

In this work, we present a novel strategy for the pre-tabulation of chemistry tables for reactive flow simulations. The approach uses locally-adaptive set of Bézier patches to map the complex chemistry. The tabulation strategy allows for an order of magnitude reduction in the table size and a user-control of the tabulation error. Given the local adaptation of the Bézier patch support points, a significant error reduction can be achieved with minimal increase in the table size. Furthermore, the search algorithm uses a hybrid approach based on a one-step quad-tree followed by a linear search which effectively decouples the table size from the total search time. A set of 100,000 queries take about one second to complete. This tabulation strategy has been successfully applied

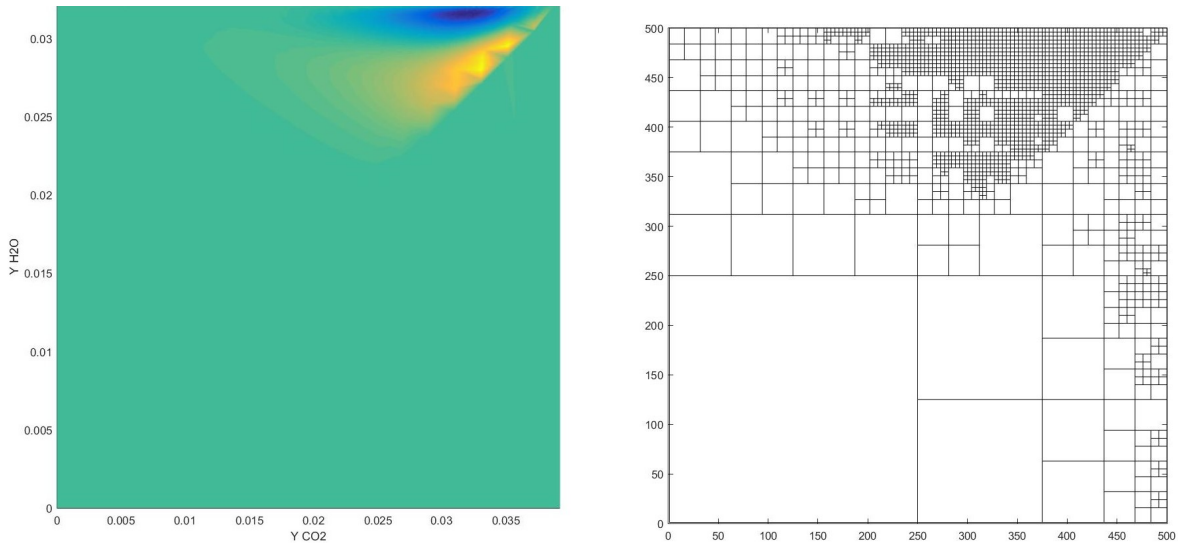

Fig. 3: Adaptive Bézier patch arrangement on the H_2 source term of the TGLDM table.

to FPVA and TGLDM tables. The drastic table size reduction affords new possibilities in high-dimensional chemistry manifolds or the consideration of additional physics (pressure variation, radiation, multi-fuels etc.). Future work will focus on Bézier hypervolumes to accurately account for the complex chemical processes which has the potential of offering an even greater reduction of tabulated chemistry size.

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