On the use of interpolating wavelets in the direct numerical simulation of combustion

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1. Motivation

Direct Numerical Simulation (DNS) of turbulent flows is an activity severely limited by presently available computer power. It has long been known (e.g. Corrsin 1961) that in order to resolve accurately the governing Navier-Stokes equations, the number of computational cells required scales as a super-linear power of the Reynolds number. Reacting systems add additional complexity to this already bleak picture. In many flows of industrial interest, the length and time scales associated with the reaction mechanism are much smaller than those of the fluid turbulence, and the resolution requirements for chemically active flow simulations are thereby considerably increased. When this is added to the computational expense incurred by the stiffness of highly non-linear reaction rate source terms, it appears that reacting flow simulations of significant complexity will remain firmly out of reach for the foreseeable future. Nonetheless, the same spatial and temporal stiffness that gives rise to such demanding computations may paradoxically provide a foothold for efficient numerical methods. Many industrial processes involving combustion occupy the *laminar flamelet regime* (Libby & Bray 1980, Bray, Libby & Moss 1985) where the turbulent flame can be regarded as a highly localized sheet of chemical activity, either side of which the fluid composition remains relatively constant.

The ability of wavelet based methods to analyze functions in terms of their *local* rates of change appears eminently suited to the numerical investigation of non-linear partial differential equations, the solutions to which often contain a large number of disparate length scales. In particular, the efficient discretization of fluid flow problems have been the focus of a number of recent investigations, both with chemical reaction (Bockhorn, Frölich & Schneider 1995, Frölich & Schneider 1996, Frölich & Schneider 1997,) and without (Bacry, Mallat & Papanicolaou 1992, Frölich & Schneider 1995, Bihari 1996). Many of the discretizations proposed to date have been limited to periodic domains although recent efforts have led to advances in non-periodic discretizations (Vasilyev, Paolucci & Sen 1995, Vasilyev & Paolucci 1996, Vasilyev & Paolucci 1997).

In this paper, we discuss the generalization to two spatial dimensions of an existing wavelet based scheme intended for combustion problems (Prosser & Cant 1998a). The approach adopts a collocation strategy but, unlike traditional collocation methods, the solution to the set of governing equations is obtained on a grid of collocation points located in a hierarchy of *wavelet* subspaces. The solution is only returned to the physical space in order to evaluate non-linear inertial and chemical reaction rate terms. The key advantage of this approach, and the motivation for its derivation, is that while the solution is expressed in terms of the wavelet spaces, it

is possible to develop an elegant algorithm to exploit the sparsity of the representation in order to reduce both the amount of storage required and the computational effort expended in resolving the chemistry fields.

2. Accomplishments

As a preliminary step towards a fully adaptive wavelet based scheme, a 2-D code has been developed. The governing equations for density, momentum, stagnation internal energy, and species mass fractions are solved using a collocation strategy. Unlike traditional collocation methods, the governing equations are satisfied at collocation points *within* the hierarchy of wavelet spaces. Due to the ability of the wavelets to identify regions of changing continuity properties, an adaption strategy based on the wavelet coefficients' absolute magnitude will automatically track the flame front during the course of a simulation.

The wavelet discretization is based on a tensor decomposition of the two dimensional computational domain and takes the form

$$\begin{aligned}\mathbf{V_J^{(2)}} &= \mathbf{V_J^x} \otimes \mathbf{V_J^y} \\ \mathbf{W_J^{(2)}} &= (\mathbf{V_J^x} \otimes \mathbf{W_J^y}) \oplus (\mathbf{W_J^x} \otimes \mathbf{V_J^y}) \oplus (\mathbf{W_J^x} \otimes \mathbf{W_J^y}) \\ &= \mathbf{W_J^{(\alpha)}} \oplus \mathbf{W_J^{(\beta)}} \oplus \mathbf{W_J^{(\gamma)}}.\end{aligned}$$

$\mathbf{V_J^{(2)}}$ and $\mathbf{W_J^{(2)}}$ are used to denote the two-dimensional scaling function and wavelet spaces, respectively. We observe that the definition of $\mathbf{W_J^{(2)}}$ involves a set of 'cross correlation' spaces, denoted here by $\mathbf{W_J^{(i)}}$, which arise via the definition of the 2-D vector space $\mathbf{V_J^{(2)}}$ and by the causal property of the multiresolution analysis: $\mathbf{V_J^{(2)}} = \mathbf{V_{J-1}^{(2)}} \oplus \mathbf{W_{J-1}^{(2)}}$. The dimensionality of the subspaces are

$$\begin{aligned}\dim(\mathbf{V_J^x} \otimes \mathbf{V_J^y}) &= (2^J + 1) \times 2^J = \dim(\mathbf{V_J^x} \otimes \mathbf{W_J^y}) \\ \dim(\mathbf{W_J^x} \otimes \mathbf{V_J^y}) &= (2^J) \times 2^J = \dim(\mathbf{W_J^x} \otimes \mathbf{W_J^y}),\end{aligned}$$

The disparity between (say) $\mathbf{V_J^x}$ and $\mathbf{V_J^y}$ arises through the span-wise periodicity in the computational domain and is discussed further in Prosser & Cant (1998a).

For this investigation, we have chosen an initial finest resolution for the computational domain of 257×64 grid points. In the language of the previous equations, this implies $\mathbf{V_J^{(2)}} = \mathbf{V_8^x} \otimes \mathbf{V_6^y}$. The reorganization of the domain under the action of the bi-dimensional wavelet transform is depicted in the lower half of Fig. 1. Note that the spanwise decomposition of the domain only occupies two subspaces while the streamwise direction employs four subspaces. This reflects the fact that the principal structure in the domain, the planar flame, is oriented with its normal initially pointing in the streamwise direction.

Figures 2 and 3 show the u-velocity surface through the flame structure and its corresponding decomposition onto a set of wavelet spaces. We see that, due to the considerable irregularity in the physical space representation of the velocity,

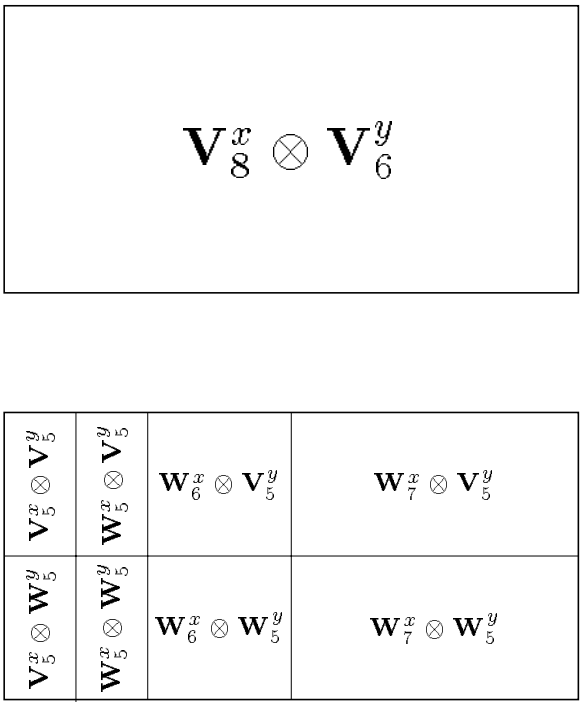

FIGURE 1. 2D tensor decomposition of initial computational domain into wavelet subspaces.

the transform domain is not sparse. This is demonstrated in Table 1 by the large number of wavelet coefficients greater than the prescribed thresholds.

Figure 4 shows a contour plot of the progress variable profile. We note that, due to the comparatively short simulation time, the degree of flame wrinkling is not great. The wrinkling that has taken place, however, is confined mainly to the preheat zone, which places the flame in the *thin reaction zones regime* discussed by Peters (1998). The considerable length scale separation between the flame structure and that of the computational domain leads to a non-trivial sparsity in the wavelet representation of the progress variable profile. Table 2 presents this sparsity in terms of the number of non-trivial wavelet coefficients measured with reference to a given datum. The table shows that, for a threshold of 10^{-5}, 85.4% of the original wavelets used to discretize the profile are redundant. The reduction in accuracy incurred by this surgery is expressed in terms of the normalized l_2 reconstruction error shown in the rightmost column of Table 2. From the small values of these errors, it is apparent that the approximation introduced by thresholding is very small.

3. Future plans

3.1 Discretization of operators

In the present formulation, the discretization of the differential operators $\frac{\partial^n}{\partial x_i^n}$ is

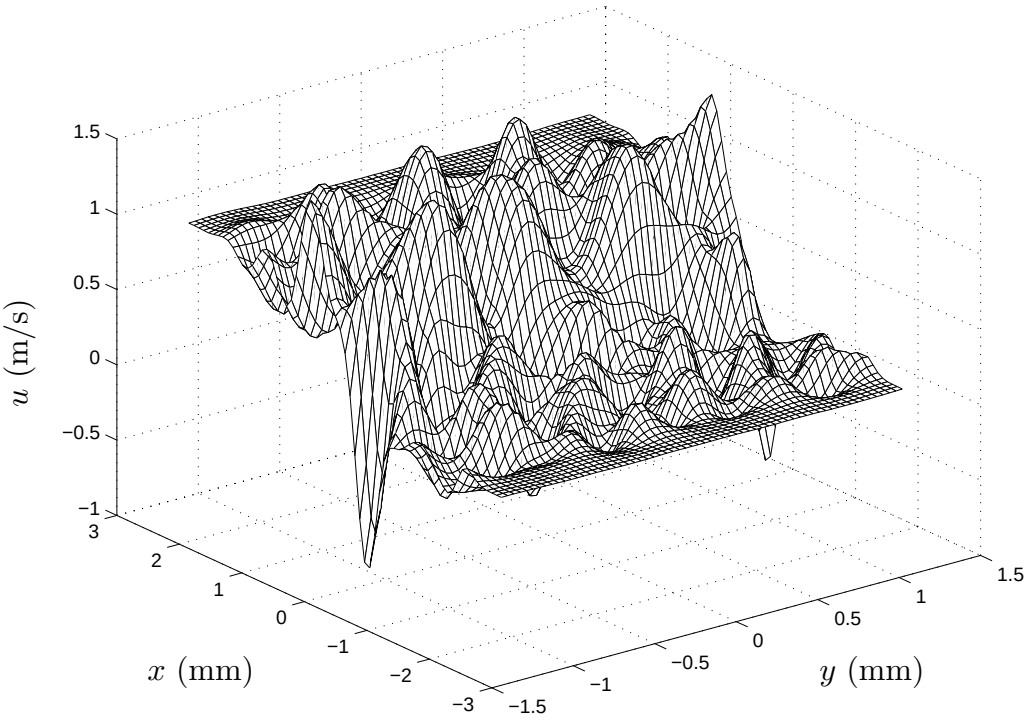

FIGURE 2. Mesh plot of u velocity in real space.

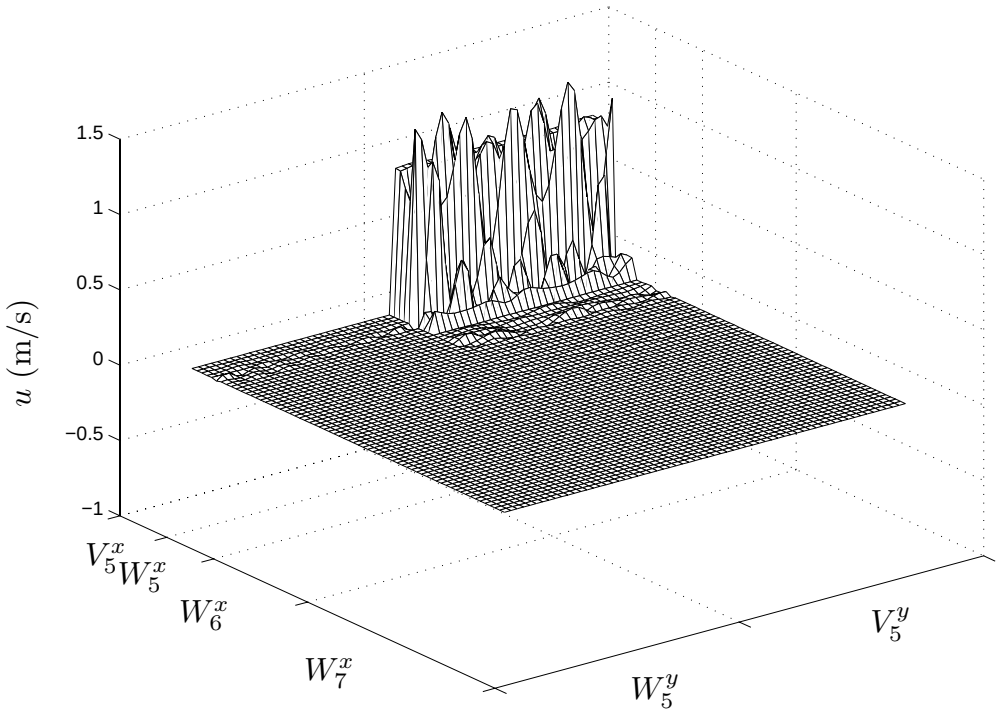

FIGURE 3. Mesh plot of u velocity in wavelet space.

ϵ	$\#\lvert d_{i,k}\rvert \geq \epsilon$	possible compression
10^{-8}	16401	1.0029
10^{-7}	15979	1.0294
10^{-6}	12734	1.2917
10^{-5}	10010	1.6432
10^{-4}	5477	3.0031

Table 1. Number of u-velocity wavelet coefficients with absolute magnitude greater than a prescribed threshold $\epsilon > 0$. Third column shows the possible compression obtainable through thresholding.

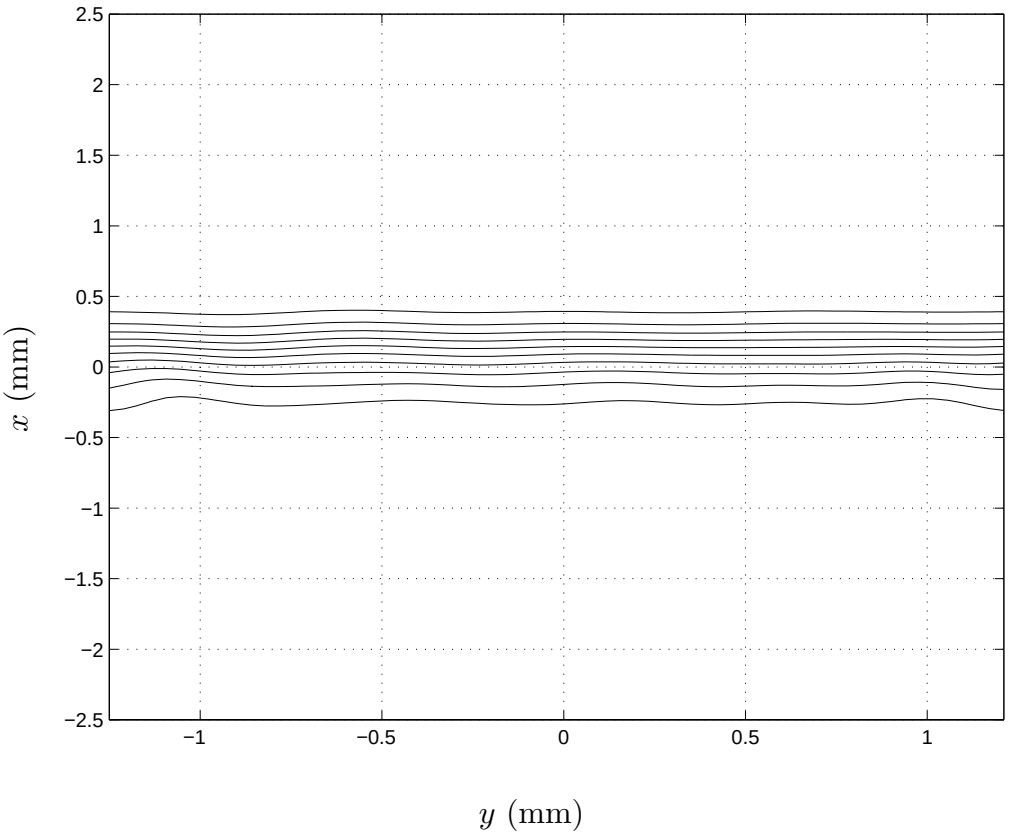

FIGURE 4. Contour plot of progress variable. Products are at the top of the plot, and reactants are at the bottom.

via the *standard decomposition*;

$$\partial_J^n = \left\{ P_{\mathbf{V_{J-p}}} + \sum_{i=J-p}^{J-1} P_{\mathbf{W_i}} \right\} \frac{\partial^n}{\partial x_i^n} \left\{ P_{\mathbf{V_{J-p}}} + \sum_{i=J-p}^{J-1} P_{\mathbf{W_i}} \right\}.$$

While this approach is the simplest to implement, it suffers from two drawbacks:

ϵ	$\#\lvert d_{i,k}\rvert \geq \epsilon$	possible compression	$\frac{\lVert c-c_\epsilon\rVert_2}{\lVert c\rVert_2}$
10^{-8}	8625	1.9070	2.3690×10^{-9}
10^{-7}	5877	2.7987	2.7555×10^{-8}
10^{-6}	4032	4.0794	2.7105×10^{-7}
10^{-5}	2407	6.8334	2.4788×10^{-6}
10^{-4}	1349	12.1297	2.8931×10^{-5}

Table 2. Number of progress variable wavelet coefficients with absolute magnitude greater than a prescribed threshold $\epsilon > 0$ and corresponding reconstruction accuracy. Third column shows the possible compression obtainable through thresholding.

- The number of non-zero coefficients in the ∂_J^n operators scale asymptotically as $\mathcal{O}(N \log_2 N)$ (Beylkin, Coifman & Rokhlin 1991).
- The structure of the operator is not readily amenable to an unbounded adaption strategy, in which an arbitrary number of discretizing nodes are introduced. Using the standard decomposition, ∂_J^n needs to be recalculated every time a new set of wavelet subspaces $\mathbf{W_J^{(2)}}$ are added or removed.

An alternate, more sophisticated approach is to represent the differential operators in terms of the *non-standard* decomposition (Beylkin, Coifman & Rokhlin 1991). In this latter technique, an arbitrary operator T can be represented as an integral kernel;

$$Tf(x) = \int k(x,y) f(y) dy.$$

The integral kernel is then expanded over a set of square wavelet subspaces (i.e. of the form $\mathbf{W_J^x} \otimes \mathbf{W_J^y}$). The advantages of this approach are twofold:

- The number of entries in the non-standard decomposition is $\mathcal{O}(N)$.
- The decomposition is self-similar across resolutions and can be implemented as a finite difference like scheme. Such an approach is much more readily amenable to truly adaptive calculations.

3.2 Evaluation of non-linear terms

The principal expense incurred using this algorithm is during the evaluation of non-linear terms. Presently, non-linearities are evaluated by first inverting the terms to physical space where, after evaluation, they are re-projected onto the hierarchy of wavelet spaces. While reasonably quick to execute, such a technique does not provide insight into the interactions between scales in the wavelet domain nor into the generation of aliasing errors.

Some preliminary work has been carried out in the evaluation of arbitrary non-linearities for one dimensional wavelet expansions (Prosser & Cant 1998b). As may be expected, the interactions produced by (say) a quadratic non-linearity introduces mixing between the subspaces occupied by the multiplicands. More importantly,

a new term is created, which cannot be represented on a fixed resolution grid and which represents the generation of un-resolvable wavelet coefficients. This term arises as a result of the increasing departure of the non-linear term from the set of polynomials spanned by the scaling function bases alone.

From a practical point of view, the new method of evaluation is approximately twice as fast in execution as the earlier method, and there are grounds for cautious optimism that this increased execution speed may scale geometrically with the spatial dimension of the problem.

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