Finite Element DVR

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I. DEFINITIONS

The finite elements are constructed by breaking space up into pieces. The boundaries of element i are defined as R^i_l and R^i_r Within each element we define a set of n_i DVR functions. The number of functions in each element is arbitrary except that we require that there be one DVR function at the boundaries. This is equivalent to requiring the Gauss quadrature to be of the Lobatto variety; two fixed points. The global basis is constructed from the set of all functions *internal* to all the elements plus the bridge functions. While it completely arbitrary, I will define the bridge function associated with the i^{th} region as,

$$\psi^i_q(x) = (f^i_N(x) + f^{i+1}_1(x)) \tag{1}$$

where f^i are the last(first) DVR functions of the i^{th} ($(i+1)^{th}$) intervals. So, by definition, the only connection between regions is via the bridge functions. The matrix elements are formed by integrating over x and summing over the regions. The contributions to matrix elements of the internal DVR functions are confined to a single element. A non-bridge function in region i connects to bridge functions at the two ends of the interval. Matrix elements between bridge functions are connected to themselves and to adjacent bridge functions. The values of the matrix elements will be computed in the next section. An important point to note about the bridge functions is that they have a discontinuous

first derivative. This requires care in computing any matrix elements involving second derivatives, which do not exist. Also, for too small a value of n_i a discontinuous derivative may lead to poor behavior of the piecewise approximation. We have not observed this in any applications to date. Clearly, there is a relationship between the size of the interval and the basis set which needs to be explored for specific problems. In practice I have observed that once one gets beyond 8 or 10 basis functions per interval, the issue of a discontinuous first derivative is no longer of practical consequence. Importantly, a judicious use of a large number of intervals and a small basis set per interval, can be quite effective in substantially reducing the number of non-zero matrix elements in a given problem. This has great import for computational techniques which rely heavily on sparse matrix manipulations.

II. MATRIX ELEMENTS

In order to avoid the problem of the non-existence of the second derivative of the bridge functions, one may formulate the problem variationally and then use Green's theorem (integration by parts) to get a variationally weak condition which avoids second derivatives. Alternatively, one may simply use an interval by interval Bloch operator approach in which the second derivative operaotr is replaced by

$$L = \frac{d^2}{dx^2} - \delta(x - R_r)\frac{d}{dx} - \delta(x - R_l)\frac{d}{dx} \tag{2}$$

We now compute the required integrals. First the overlaps. For non-bridge functions,

$$O^i_{n,m} = \int_{R_l}^{R_r} dx f^i_n(x) f^i_m(x) = w^i_n \delta_{n,m} \tag{3}$$

and for the bridge functions,

$$O^i = \int_{R_l}^{R_r} dx (f^i_N(x) + f^{i+1}_1(x))(f^i_N(x) + f^{i+1}_1(x)) = O^i_{N,N} + O^{i+1}_{1,1} = w^i_N + w^{i+1}_1 \tag{4}$$

So, all the overlaps are diagonal, as expected. Now, turn to the L matrix elements. The non-bridge matrix elements are,

$$L^i_{n,m} = \int_{R_l}^{R_r} dx f^i_n(x) L f^i_m(x) = w^i_n f''^i_m(x^i_n) \tag{5}$$

The matrix elements between a non-bridge and bridge function are,

$$\begin{aligned} L^{i,i}_{n,m} &= \int_{R_l}^{R_r} dx f^i_n(x) L(f^i_N(x) + f^{i+1}_1(x)) \\ &= L^i_{n,N} \\ L^{i,i-1}_{n,m} &= \int_{R_l}^{R_r} dx f^i_n(x) L(f^i_1(x) + f^{i-1}_N(x)) \\ &= L^i_{n,1} \end{aligned} \tag{6}$$

Finally, the bridge-bridge matrix elements are,

$$\begin{aligned} L^{i,i} &= \int_{R_l}^{R_r} dx (f^i_N(x) + f^{i+1}_1(x)) L(f^i_N(x) + f^{i+1}_1(x)) \\ &= L^i_{N,N} + L^{i+1}_{1,1} \\ L^{i-1,i} &= \int_{R_l}^{R_r} dx (f^{i-1}_N(x) + f^i_1(x)) L(f^i_N(x) + f^{i+1}_1(x)) \\ &= L^i_{1,N} \\ L^{i+1,i} &= \int_{R_l}^{R_r} dx (f^{i+1}_N(x) + f^{i+2}_1(x)) L(f^i_N(x) + f^{i+1}_1(x)) \\ &= L^{i+1}_{N,1} \end{aligned} \tag{7}$$

III. PRACTICALITIES

Let us work out the basic integral.

$$
\begin{aligned}
L^i_{n,m} &= \int_{R_l}^{R_r} dx f^i_n(x) L f^i_m(x) \\
&= w^i_n f^i_n(x_n) \frac{d^2 f^i_m(x)}{dx^2} \mid_{x_n} - f^i_n(R_l) f'^i_m(x) \mid_{R_l} + f^i_n(R_r) f'^i_m(x) \mid_{R_r}
\end{aligned}
\tag{8}
$$

Note, that the surface terms vanish unless one of the functions is at the end or beginning of the interval