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Hypergeometric Summation Techniques for High Order Finite Elements

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The goal of this paper is to discuss the application of computer algebra methods in the design of a high order finite element solver. The finite element method is nowadays the most popular method for the computer simulation of partial differential equations. The performance of iterative solution methods depends on the condition number of the system matrix, which itself depends on the chosen basis functions. A major goal is to design basis functions minimizing the condition number, and which can be implemented efficiently. A related goal is the application of symbolic summation techniques to derive cheap recurrence relations allowing a simple and efficient implementation of basis functions.

1 Finite Element Method

Many problems in science and engineering are described by partial differential equations. To solve these equations on non-trivial domains, numerical methods such as the finite element method are required. We are interested in solving variational boundary value problems (BVP) posed in some Sobolev space. Via discretization the problem of solving the variational BVP becomes the problem of solving a linear system $Au = f$. In the finite element method (FEM) the domain of interest is divided into a mesh consisting of (possibly curved) triangular, quadrilateral (2D), tetrahedral, prismatic, pyramidal and hexahedral (3D) elements. On this mesh one defines a basis of locally supported, piecewise polynomial functions.

The two main philosophies in the FEM are the h- and the p-version. In the h-version the mesh is refined in order to achieve a better accuracy, keeping the basis functions on a fixed low degree (usually linear). Whereas in the p-version one computes on a fixed coarse mesh and increases the polynomial degree of the basis functions to obtain a better result. Here h corresponds to the mesh-size and p to the maximal polynomial degree. The high-order approach (i.e. the p-version) is suitable especially when the solution of the problem is smooth.

The combination of the two strategies is called the hp-method, where the mesh is refined towards singularities. On the elements with small diameter the basis functions are of low degree and on the coarser parts of the mesh one computes with high-order elements.

2 Construction of high order finite elements

In general computations are performed on some reference element and are then transformed to the actual element in the mesh, so for the construction we restrict ourselves to some reference element. First let us consider basis functions in 1D. Here the elements are simply intervals over the real line and usually one chooses hierarchic shape functions on the reference element $(-1, 1)$,

$$\varphi_0(x) = \frac{1+x}{2} \qquad \varphi_1(x) = \frac{1-x}{2} \qquad \varphi_i(x) = (1-x^2)\psi_{i-2}(x) \quad \text{with} \quad \psi_{i-2} \in P^{i-2}(-1,1).$$

The interior bubbles $\varphi_i,\ i \geq 2$, vanish at the endpoints ± 1 and are products of $(1-x^2)$ and a polynomial ψ_{i-2} of degree $i-2$. Most often the ψ_i are chosen to be orthogonal polynomials such as Jacobi polynomials $P_i^{(\alpha,\beta)}(x)$ which are orthogonal w.r.t. the weighted scalar product $(p,q) = \int_{-1}^{1}(1-x)^\alpha(1+x)^\beta p(x)q(x)\,dx$. One reason why orthogonal polynomials are preferred is because they are efficiently computable by 3 term recurrences, i.e.

$$\psi_i(x) = (a_i + b_i x)\psi_{i-1}(x) + c_i\psi_{i-2}(x), \qquad i \geq 1,\ \psi_0(x) = 1,\ \psi_{-1}(x) = 0. \tag{1}$$

The recurrence coefficients a_i, b_i, c_i are rational functions in i (see e.g. [1]). To illustrate the construction of 2D-basis functions let us first consider quadrilateral elements. Again we choose hierarchic shape functions on the reference square $(-1,1)^2$. Usually one exploits the tensor product structure of quadrilateral elements and defines the basis functions on quadrilaterals as tensor products of the 1D basis functions, i.e.

$$\phi_{i,j}(x,y) = \varphi_i(x)\varphi_j(y), \qquad x, y \in (-1,1),\ i,j \geq 0.$$

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In 2D one distinguishes between vertex, edge and inner basis functions. Vertex basis functions equal 1 on the defining vertex and vanish on the other vertices, egde based basis functions are polynomials on the defining edge and zero on all other edges and interior bubbles vanish on the boundary of the element. Also for triangles one uses a tensor-product-structure [4] by collapsing the quadrilateral to the triangle using the map $x \mapsto (1-y)x$. The definition of high order elements in three dimensions follows the same principle and yields also basis functions in tensor product structure.

3 Linking Symbolic to Numerical Computations

As mentioned at the beginning of this paper, the problem of solving a PDE is transformed into the problem of solving a linear system $Au = f$, where the system matrix A is e.g. $A_{i,j,k,l} = \iint_\Omega \nabla\phi_{i,j}(x,y)\nabla\phi_{k,l}(x,y)\,d(x,y)$. This equation system is usually large scaled, so one uses iterative procedures to solve it. For the iterative solvers we want basis functions with good numerical properties, i.e. they generate a sparse system matrix with a small condition number and allow fast integration.

One possibility to implement fast integration is to use the three term recurrence (1). Let $\Psi_{i,j} = \int_{-1}^{1}\gamma(x)\psi_i(x)\psi_j(x)$, where $\gamma(x)$ is some coefficient function. We can think of $\Psi_{i,j}$ as the entries of a matrix Ψ and, as we are using tensor products for the basis functions in 2D and 3D, the building blocks of the system matrix are of this type. We have deduced the following x-free recurrence for the matrix entries $\Psi_{i,j}$,

$$\Psi_{i+1,j} = \frac{a_{i+1}b_{j+1} - b_{i+1}a_{j+1}}{b_{j+1}}\Psi_{i,j} + \frac{b_{i+1}}{b_{j+1}}\Psi_{i,j+1} - \frac{b_{i+1}c_{j+1}}{b_{j+1}}\Psi_{i,j-1} + c_{i+1}\Psi_{i-1,j}.$$

So having a recurrence for the basis functions (or factors of them) allows implementing a fast integration procedure.

We will conclude this article by briefly describing our construction of new basis functions related to edges which provide a good behavior w.r.t. the condition number of the system matrix and for which the CA procedures of P. Paule, A. Riese and C. Schneider could find a 5-term recurrence. A more detailed description can be found in [3].

Example: Low Energy Based Basis Functions on Triangles. We start our construction with a polynomial defined on the lower edge of the reference triangle $\{(-1,0),(1,0),(0,1)\}$, vanishing in ± 1. In a first step we define an extension on the interior of the triangle by $\phi_i^{(1)}(x,y) = \frac{1}{2y}\int_{x-y}^{x+y}\varphi_i(s)\,ds$, similar to [2]. This extension does not yet provide homogenous boundary conditions, which is fixed by linear interpolation between the lower and the upper two edges. Accordingly we define

$$\phi_i(x,y) = \phi_i^{(2)}(x,y) - \frac{y}{z_2}\,\phi_i^{(2)}(z_2-1,z_2), \quad \text{where} \quad \phi_i^{(2)}(x,y) = \phi_i^{(1)}(x,y) - \frac{y}{z_1}\,\phi_i^{(1)}(1-z_1,z_1),$$

$z_1 = (1-x+y)/2$ and $z_2 = (1+x+y)/2$. With the aid of the RISC summation packages, in particular C. Schneider's Sigma [6] and C. Mallinger's Generation Functions package [5], we have derived the following recurrence for the $\phi_i(x,y)$,

$$\phi_i = a_i x\phi_{i-1} + (b_i + c_i(x^2-y^2))\phi_{i-2} + d_i x\phi_{i-3} + e_i\phi_{i-4}, \qquad i \geq 6$$

with the coefficients $a_i = \frac{2(2i-3)}{(i+1)}$, $b_i = -\frac{(2i-5)(3-10i+2i^2)}{i(i+1)(2i-7)}$, $c_i = -\frac{(2i-5)(21-20i+4i^2)}{i(i+1)(2i-7)}$, $d_i = \frac{2(i-5)(2i-3)}{i(i+1)}$ and $e_i = -\frac{(i-6)(i-5)(2i-3)}{i(i+1)(2i-7)}$. This was accomplished by first representing ϕ_i in hypergeometric sum notation yielding a term that can be split into three sums, one of which simplifies to zero (proof by Sigma). For the remaining two sums Sigma provides recurrence formulas which then can be added using the **RecurrencePlus** command of Generating Functions.

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