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The spectral element method for static neutron transport in A_N approximation. Part II

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To Mike, in deep appreciation of the mathematical elegance he has consistently brought to the science of particle transport.

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ABSTRACT

This paper is the second part of an investigation on the use of the spectral element method (SEM) to solve neutron transport problems in the A_N approximation. Part I of the study contained a description of the SEM variational approach of the A_N equations applied to classical assembly benchmark problems. Part II deals with the SEM solution of these equations in reactor cells. To cope with the cell geometry we apply a mapping technique from curved to square domains based on transfinite interpolation. Benchmark exercises – based on the method of characteristics – on the scale of fuel cells give a further confirmation of the computation advantages of the SEM-A_N approach in comparison with classical low-order computational techniques.

1. Introduction

This paper is the second part of an investigation on the use of the spectral element method (SEM) to solve two-dimensional neutron transport problems in the variational formulation of the A_N approximation (Barbarino et al., 2013; Ciolini et al., 2002). In the first part of the study we developed the SEM method in continuous and discontinuous Galerkin approaches and we applied the technique to the solution of some classical reactor benchmark problems. The results showed that accurate solutions could be obtained for the Natelson and the IAEA-EIR2 benchmark configurations (Natelson, 1971; Khalil, 1985). Interesting features were highlighted and the method looked quite efficient for transport computations in full-core nuclear systems. Further evidence of the merits of SEM, compared to the classical finite difference (FD) and diamond difference (DD) schemes were given in a recent study involving polynomial and non-polynomial manufactured solutions on standard domains (Barbarino et al., 2014). Clearly, combining high-order spectral elements for the space variable and S_N methods for the angular dependance, one is able – in these highly unrealistic circumstances – to reduce the computation errors to round-off level by careful selection of the polynomial degree for the space variables, and of the angular order N.

In this companion paper the investigation is carried one step further to assess the merits of the method when solving the A_N formulation of the linear transport equation with more complex geometries involving the presence of curved boundaries, as for a single core cell made of a fuel pin with cladding surrounded by a moderator. A tricky aspect of the computation lies in the geometry, the circular fuel pin and cladding being embedded in a square domain. To avoid spoiling the accuracy of the SEM discretization, it is utterly important to reproduce exactly the circular boundary between the cladding and the moderator in the partitioning of the domain. This is made possible through the use of a mapping technique based on transfinite interpolation. In a previous work performed by Bjontegaard et al. (2012) the Poisson equation has been solved on deformed domains adopting different mapping techniques and proving that the exponential error decay characteristics of SEM can be preserved. In this work, the application of transfinite interpolation is extended to the peculiar geometry considered for lattice calculations in reactor physics simulations, testing the performance of SEM against a standard FEM approach.

As the interpolation technique plays a central role in the implementation of the spectral element method on a reactor cell and to similar domains where curved boundaries are present, Section 2 is dedicated to its basic principle. Notice that, with regard to the

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other aspects, namely the variational approach in continuous and discontinuous Galerkin formulation, all details – up to the construction of the algebraic system and its solution using preconditioned iterative methods – may be found in the companion paper and hence will only briefly be recalled here.

Section 3 is dedicated to the discussion of several numerical tests. Results obtained with spectral elements and A_N are compared with classical low-order methods and the method of characteristics for benchmark purposes. Finally, Section 4 draws the conclusion.

2. Application of spectral elements to complex geometries

Application of SEM is straightforward when the integration domain is the union of quadrangles. It becomes more complicated – though tractable – when the geometry includes curved subdomains, which includes for instance the case of a nuclear fuel cell in reactor calculations. The basic constraint lies in the fact that, in any mapping, curved boundaries must be reproduced in the *continuous sense*. Consider Fig. 1 where a 2D reference domain $\hat{\Omega} := [-1,+1]^2$ is transformed into the domain Ω through the transformation $\Gamma = (x(s,t), y(s,t))$. In practice Ω is imposed, depending on the geometry of the problem. One is looking therefore in fact for Γ^{-1}, which might be almost impossible to obtain in compact analytical form, except in some special cases. The transfinite interpolation technique due to Birkhoff, Gordon and Hall (1973) is a convenient and accurate approximation technique allowing to deal with the problem. The technique does not provide the Γ transformation but a Lagrangian interpolation of Γ with interpolation property satisfied on the whole contour of $\hat{\Omega}$, that is a one-to-one correspondence between the boundaries of Ω and $\hat{\Omega}$. The evaluation of the Jacobian matrices and metrics to build the SEM mass and stiffness matrices in the Ω domain becomes then straightforward (Barbarino, 2014). In the following we will describe the methodology in two space dimensions. The reader should notice that it is easily extended to 3D.

2.1. The 2D transfinite mapping technique

Consider the one-dimensional reference domain $\hat{\mathcal{O}} := [-1,+1]$ and let P_x denote the linear Lagrangian interpolation operator on $\hat{\mathcal{O}}$. This implies that $f_I(x)$, linear Lagrangian interpolation of any suitable function $f(x)$, writes:

$$f_I(x) := P_x f(x) = f(-1)\,\vartheta_1(x) + f(1)\,\vartheta_2(x), \tag{1}$$

with

$$\vartheta_1(x) = \frac{1-x}{2}, \quad \vartheta_2(x) = \frac{1+x}{2}. \tag{2}$$

The interpolation error distribution may be represented by an operator Q_x acting on $f(x)$ such that

$$\varepsilon(x) = f(x) - f_I(x) = (I - P_x)f(x) = Q_x f(x), \tag{3}$$

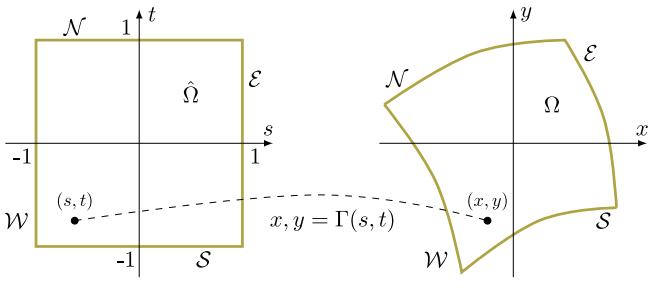

Fig. 1. Deformation of a reference element.

where I denotes the identity operator. As is well known, this error decreases quadratically in terms of the interpolation mesh as this goes to zero:

$$\|\varepsilon(x)\| \approx O(h^2). \tag{4}$$

Consider now the two-dimensional reference domain $\hat{\Omega} := [-1,+1]^2$ and P_x and P_y the one-dimensional linear Lagrangian interpolation operators in x and y respectively. Intuitively, the most natural extension of the interpolation process in two space dimensions is based on the use of the tensor product, whereby:

$$f_I^{tp}(x,y) := P_x P_y f(x,y). \tag{5}$$

Here, the associated interpolation error distribution is

$$\begin{aligned}\varepsilon^{tp}(x,y) &= f(x,y) - f_I^{tp}(x,y) = (I - P_x P_y)f(x,y)\\ &= (Q_x + Q_y - Q_x Q_y)f(x,y),\end{aligned} \tag{6}$$

the last relationship being obtained by substitution of P_x and P_y by respectively $I - Q_x$ and $I - Q_y$. Obviously the error reduction will be of the same order as in the one-dimensional case since, according to (6),

$$\|\varepsilon^{tp}(x,y)\| \approx O(h_x^2) + O(h_y^2), \tag{7}$$

where h_x and h_y denote the interpolation meshes in the x and y variables.

The operators P_α and Q_α ($\alpha = x, y$) are complementary since by definition $P_\alpha + Q_\alpha = I$. Hence, if one adopts the two-dimensional interpolation scheme

$$f_I^{bs}(x,y) := (P_x + P_y - P_x P_y)f(x,y) := P_x \oplus P_y f(x,y) \tag{8}$$

rather than the tensor product, the associated interpolation error distribution automatically writes:

$$\begin{aligned}\varepsilon^{bs}(x,y) &= f(x,y) - f_I^{bs}(x,y) = (I - P_x \oplus P_y)f(x,y)\\ &= Q_x Q_y f(x,y).\end{aligned} \tag{9}$$

The error norm in this case should be much smaller than the previous one since, due to (9):

$$\|\varepsilon^{bs}(x,y)\| \approx O(h_x^2 h_y^2). \tag{10}$$

The two-dimensional interpolation operator $P_x \oplus P_y$ of Eq. (8) is the *Boolean sum* of the one-dimensional operators P_x and P_y. In expanded form, one writes:

$$\begin{aligned}f_I^{bs}(x,y) = {} & f(-1,y)\vartheta_1(x) + f(1,y)\vartheta_2(x) + f(x,-1)\vartheta_1(y)\\ & + f(x,1)\vartheta_2(y) - f(-1,-1)\vartheta_1(x)\vartheta_1(y)\\ & - f(-1,1)\vartheta_1(x)\vartheta_2(y) - f(1,-1)\vartheta_2(x)\vartheta_1(y)\\ & - f(1,1)\vartheta_2(x)\vartheta_2(y).\end{aligned} \tag{11}$$

The enhanced accuracy (10) is due to the fact that the Boolean sum interpolation operator $P_x \oplus P_y$ reproduces the function $f(x,y)$ *exactly* along the four edges of the reference domain $\hat{\Omega}$. Indeed, one can easily verify using (8) that the following four identities hold:

$$f_I^{bs}(\pm 1, y) = f(\pm 1, y) \quad \text{and} \quad f_I^{bs}(x, \pm 1) = f(x, \pm 1). \tag{12}$$

This transfinite interpolation property is precisely what is needed to superpose a spectral element grid on a curved domain.

As mentioned before, the two-dimensional domain mapping problem consists in finding two functions $x(s,t)$ and $y(s,t)$ constituting the components of the transformation $\Gamma(s,t)$ between $\hat{\Omega}$ and Ω. The use of the transfinite technique consists in looking for the Boolean interpolated functions $x^{bs}(s,t)$ and $y^{bs}(s,t)$ of the transformation, $\Gamma^{bs}(s,t)$, instead of identifying the transformation Γ. To this aim, it is necessary to know the law $\{s,t\} \to \{x,y\}$ for each of