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THE HIGH ORDER FINITE ELEMENT METHOD FOR STEADY CONVECTION-DIFFUSION-REACTION PROBLEMS (ECCOMAS CFD 2010)

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Abstract: *A wide class of mass transfer problems is governed by the combined effect of convection, diffusion and reaction (CDR) processes. The finite element method using the standard Bubnov Galerkin method based on linear elements is widely applied for diffusion-dominated problems where the method produces accurate results. However, at high Péclet numbers of transport problems, where the convection process dominates, this scheme gives rise to numerical oscillations in the solution which do not coincide with the physical phenomena. As a remedy, the high order finite element method is applied for CDR problems in this paper. Two numerical examples are taken as test cases to illustrate the capability of the high order finite element method of suppressing residual oscillations. An error convergence study is also presented to show the different characteristics of the convergence of h-refinement and p-refinement.*

1 INTRODUCTION

In groundwater flow, the distribution of a substance which is fully dissolved in the medium can be affected by three factors in the transportation: convection, diffusion and reaction. It is well known that pure diffusion flow problems can be accurately solved by the standard Bubnov Galerkin finite element method. However, when the convection behaviour of the flow becomes dominant, the finite element method using the standard Bubnov Galerkin scheme based on linear elements exhibits numerical oscillations in the solution. The underlying reason is that the inclusion of the convective term in the stiffness matrix gives rise to complex eigenvalues of the stiffness matrix, which mathematically contributes an oscillation component to the solution.

One effective stabilisation-scheme proposed to prevent the numerical oscillation is the SUPG (Streamline-upwind Petro-Galerkin) [2] method. The SUPG method can eliminate the oscillation in the solution by introducing the modified weighting function in the equation, being different from the unknown function. The main complexity of this method is to model the perturbation terms – an additional numerical diffusivity – to enhance the numerical stability.

In this paper, a numerical study of the steady-state distribution of a substance is presented with higher order finite elements using the standard Bubnov Galerkin method. The simplicity of forming weighting functions benefiting from the standard Bubnov Galerkin method is maintained and the oscillation of the solution is reduced by increasing the polynomial degree of the shape functions. In contrast to *h*-FEM, where the accuracy in the solution is improved by the refinement of the mesh, the high order finite element method (also called *p*-FEM) achieves the convergence of the unknowns by increasing the order of shape functions for a fixed mesh. This method is also discussed in the book of Donea and Huerta [3] in comparison with *h*-FEM. In this book, quadratic elements are applied for an one-dimensional convection dominated problem and the conclusion is "…as the Péclet number is increased beyond unity, the solution has a boundary layer, which cannot be resolved by the standard Bubnov Galerkin method…", which is also a common perception. This statement is further discussed in this paper, and the possibility of utilising the standard Bubnov Galerkin method is pointed out.

2 MATHEMATICAL MODEL

The transport equation of the convection-diffusion-reaction problem is derived based on the mass conservation law in fluid dynamics. Accordingly, for a steady-state problem, a substance in a control volume is conservative by the balance between the amount of the substance entering and leaving the control volume and the contributions from the source or the sink of that substance. The amount of the substance entering and leaving a control volume, which is called flux, is composed of convective flux, transported by the flow, and diffusive flux that is induced by molecular collisions. A chemical reaction may occur as well during the transportation process, which leads to the differential equation of the steady transport [1].

$$a \cdot \nabla c - \nabla \cdot (\nu \nabla c) + \sigma c = f \tag{1}$$

Here, a is the given velocity field, c is the unknown concentration of a substance, ν is the diffusion coefficient, σ is the reaction coefficient, and f is the source function in the control volume.
To characterise the relative importance of the convection and diffusion, the Péclet number is introduced which expresses the ratio between diffusive flux and convective flux. The mesh Péclet number is a dimensionless number where the characteristic length of the mesh size *h/2* is included. It is defined as:

$$Pe = ah/2\nu \tag{2}$$

When the convective flux dominants, the Péclet number becomes larger than 1. Consequently, the truncation error from the Galerkin method based on linear elements is not negligible any more since it is a function of Pe and the magnitude of the truncation error increases with a growing Pe [3]. This is the reason why convection dominated flow produces oscillation in the standard Bubnov Galerkin finite element method.
In finite element methods, the weak form of the partial differential equation (1) is required for the discretization of the equation system. After multiplying the weighting function w to both sides of Equation (1), the integration by parts for the diffusive term leads to:

$$\int_{\Omega} [a \cdot (\nabla c) \cdot w + (\nabla c) \cdot \nu \cdot (\nabla w) + \sigma \cdot c \cdot w] dv = \int_{\Omega} (f \cdot w) dv \tag{3}$$

The exact solution c_{EX} is then approximated by an ansatz, which is the linear combination of the shape functions with polynomial degrees up to *p*.

$$c_{FE} = \sum_{i=1}^{p+1} N_i c_i \tag{4}$$

In Equation (4), c_{FE} is the approximation of the exact solution in the finite element space while N_i and c_i represent the shape functions and the coefficients that determine the weight of the shape functions in the approximation respectively [4]. The dimension of the space V depends on the number of linearly independent shape functions, and therefore, the approximation space can be expanded by increasing the polynomial degree *p*. This basic concept of *p*-FEM is applied in the next two examples.

3 NUMERICAL EXAMPLES

3.1 One-dimensional convection-diffusion problem

In this section, numerical results of the one-dimensional convection-diffusion transport problem are compared to the exact solution. The differential equation

$$a \cdot \frac{d^2 c}{dx^2} - \nu \cdot \frac{dc}{dx} = 0 \tag{5}$$

has the following boundary condition in $\Omega = (0,1)$: $c(x = 0) = 0, c(x = 1) = 1$, and it has the exact solution:

$$x = \frac{1-\exp(\frac{ax}{\nu})}{1-\exp\left(\frac{a}{\nu}\right)} \tag{6}$$

When the mesh is fixed, the ratio between the velocity and the diffusivity determines the Péclet number as well as the convergence of the numerical solution. When the Péclet number increases, the standard Bubnov Galerkin method based on linear elements exhibits oscillations in the numerical solution. Figure 1, 2, and 3 show numerical solutions with three different Péclet numbers, using 10 linear elements with $h = 0.1$. The dashed line denotes the exact solution while the solid line represents the numerical solution.

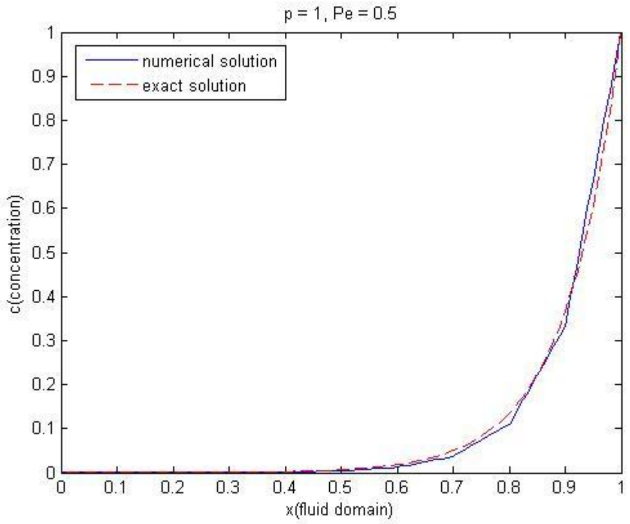


Figure 1: The numerical and the exact solution with *Pe* = 0.5 using linear elements

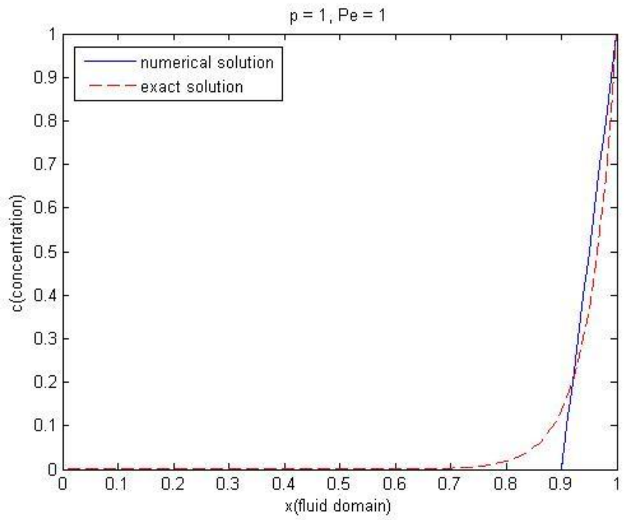


Figure 2: The numerical and the exact solution with *Pe* = 1 using linear elements

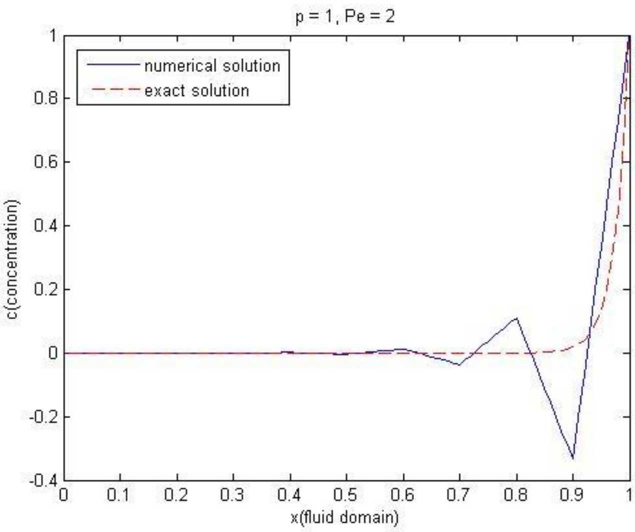


Figure 3: The numerical and the exact solution with *Pe* = 2 using linear elements

As expected, when the Péclet number is larger than 1, the solution starts to oscillate. If the velocity is zero, it is a pure diffusion problem with *Pe* = 0, and thus the stiffness matrix is symmetric, whose eigenvalues are all real. However, when the velocity is bigger than zero, the convection term starts to add a non-symmetric matrix component to the system matrix. When the number of Péclet is larger than 1, the eigenvalues of the system matrix are complex, where the nonzero imaginary part of the eigenvalues contributes the oscillatory component to the solution.
The performance of the *p*-FEM is further investigated in the next example. We choose the following parameters: $a = 100, v = 1, Pe = 5$. The corresponding numerical solutions are obtained with 10 elements in the same length. Figure 4, 5, and 6 show the comparison between the exact solution and the numerical solution for different polynomial degrees.

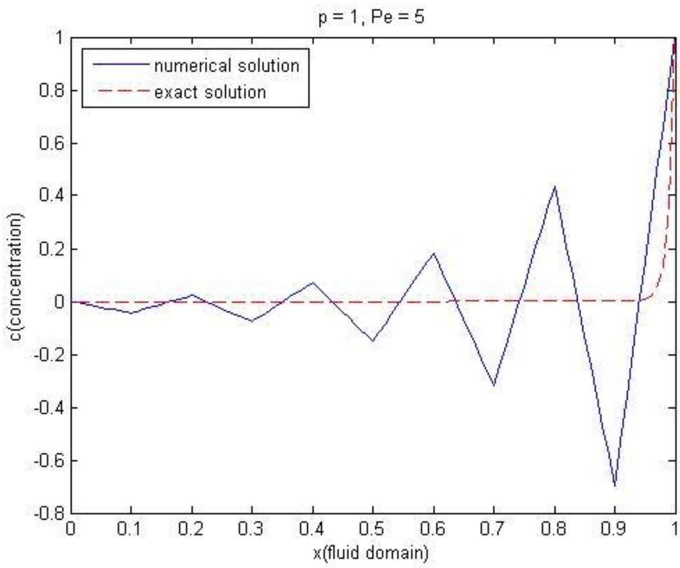


Figure 4: The numerical and the exact solution with *p* = 1, *Pe* = 5

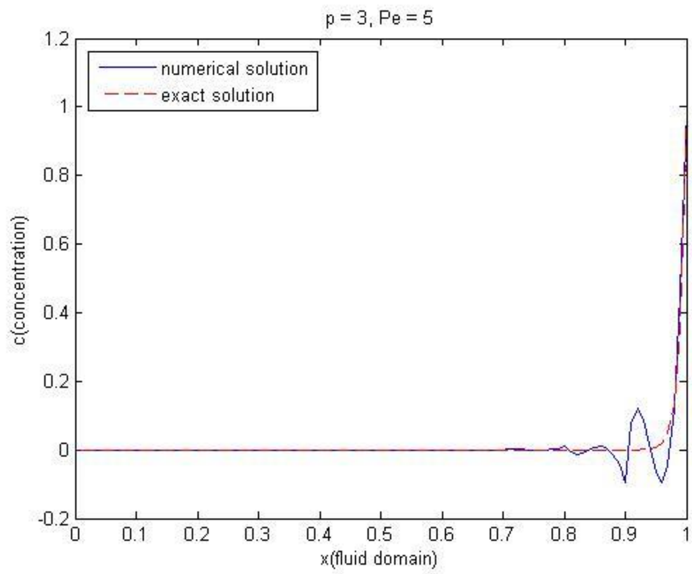


Figure 5: The numerical and the exact solution with *p* = 3, *Pe* = 5

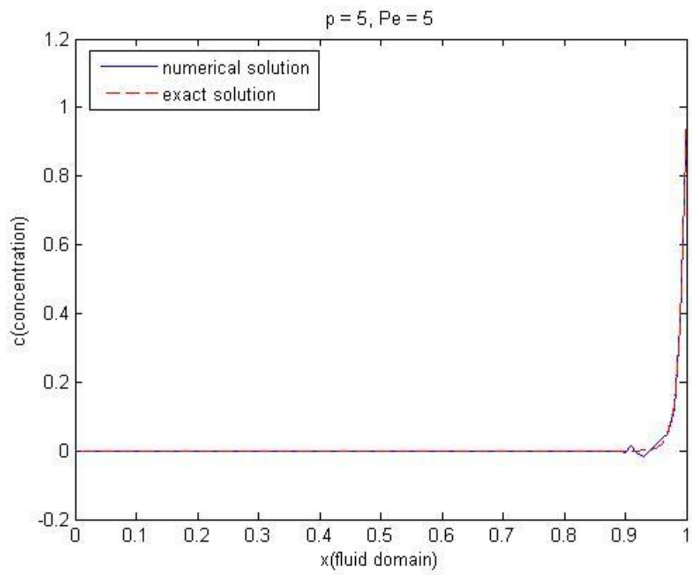


Figure 6: The numerical and the exact solution with *p* = 5, *Pe* = 5

Obviously, the oscillation tends to decrease as the polynomial degree of the ansatz is increased. With *p*=5, the numerical solution is in good agreement with the exact solution.

3.2 Two-dimensional steady rotating pulse problem

This test case investigates a two-dimensional diffusion-convection-reaction transport problem with a rotating velocity and a discontinuous source. The differential equation of the problem is equivalent to Equation (1). It has following boundary conditions in $\Omega = (-1,1) \times (-1,1) : c(x = -1) = c(x = 1) = c(y = -1) = c(y = 1) = 0$.
Here, the velocity field is given as:

$$a = \phi(\rho)\begin{pmatrix} -y \\ x \end{pmatrix}$$

$$\phi(\rho) = \begin{cases} 1-\rho^2 & if\ \rho \leq 1 \\ 0 & else \end{cases} \tag{7}$$

$$\rho = \sqrt{x^2 + y^2}$$

The magnitude of the velocity over the domain is depicted in Figure 7.

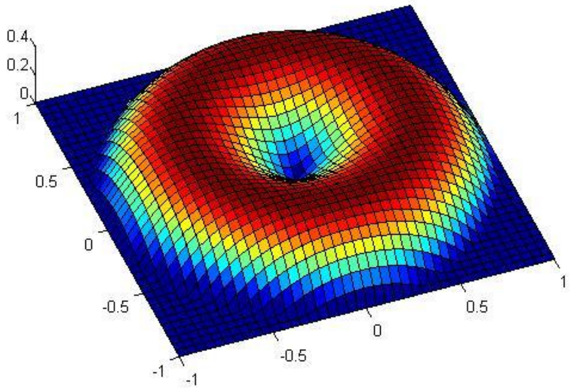


Figure 7: The magnitude of the velocity field

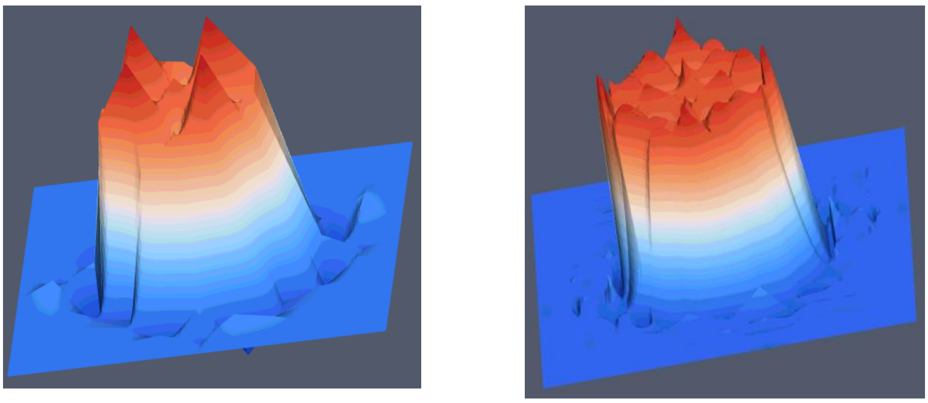
For the following computations, the coefficients are defined as follows:

$$\sigma = 2$$

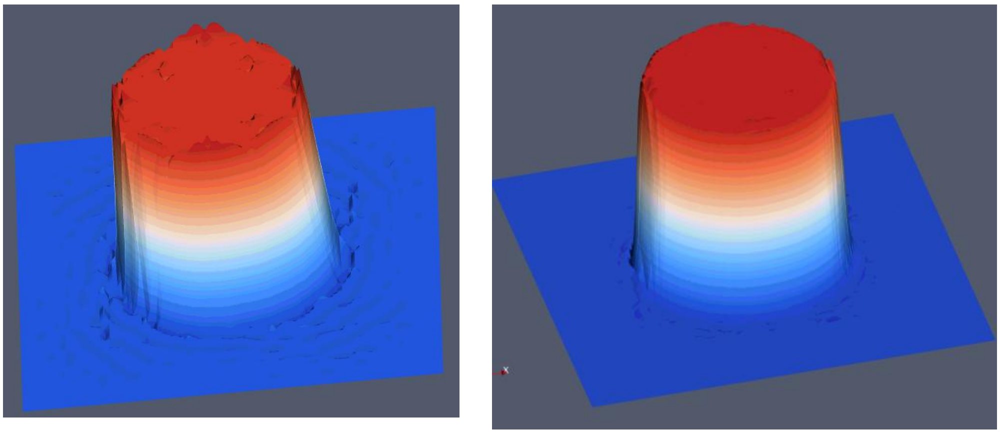
$$\nu = 0.0001 \tag{8}$$

$$s = \begin{cases} 1 & if\ \rho \leq 1/2 \\ 0 & else \end{cases}$$

This example is also discussed in the book of Donea and Huerta [3] and the result has a boundary layer along the circle $\rho = 1/2$. Here, a uniform mesh with 10 times 10 elements is applied and the numerical solution based on different polynomial degrees of the ansatz can be observed in Figure 8.



$p = 1$ $p = 3$



$p = 6$ $p = 12$

Figure 8: The numerical solutions with different polynomial degrees

The numerical result has a strong oscillation along the boundary layer with the application of linear elements. This numerical oscillation can be suppressed by increasing the polynomial degree of the ansatz shown in Figure 8. One can see that *p*-FEM with the standard Bubnov Galerkin method is also capable of resolving the solution with a boundary layer.

4 ERROR ANALYSIS

The numerical error in the finite element approximation can be quantified by the error in the energy norm. The error is defined by

$$e = c_{EX} - c_{FE} \tag{9}$$

And the error in the energy norm is defined by

$$\|e\|_{E(\Omega)} = \sqrt{\frac{1}{2}\int_{\Omega} \left(a \cdot (\nabla e) \cdot e + (\nabla e) \cdot \nu \cdot (\nabla e) + \sigma \cdot e \cdot e\right) dv} \tag{10}$$

Let us take the one-dimensional convection-diffusion problem as an example. The error in the energy norm is computed with different Péclet numbers and different polynomial degrees. The result is plotted in Figure 9 with a logarithmic scale.

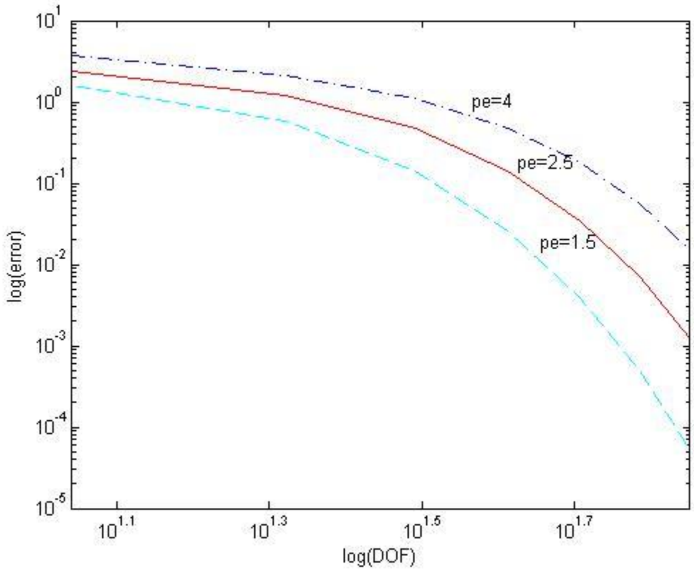


Figure 9: Error in the energy norm with different Péclet numbers

Figure 9 shows the exponential convergence of the error in the energy norm when the degrees of freedom increase by pure *p*-extension. The effect of the Péclet number can also be observed in this figure. The convergence ratio of *p*-FEM is compared with *h*-FEM for one-dimensional problem with the Péclet number 1.5 in Figure 10. The solution obtained by *p*-refinement has a faster convergence in this case than the algebraic one given by *h*-refinement with the application of the standard Bubnov Galerkin method.

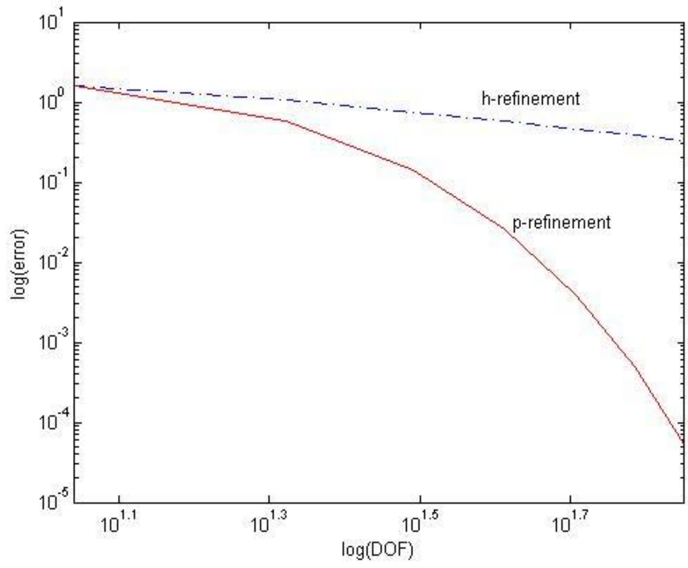


Figure 10: The convergence speed of *h*-refinement and *p*-refinement

5 CONCLUSIOINS

In this paper, the high order finite element method with the standard Bubnov Galerkin method is applied for convection-diffusion-reaction flow problems. It is a well known fact that the Bubnov Galerkin method leads to artificial oscillations for convection dominated problems of this type in case low order finite elements are used.

It is a common perception that high order finite element methods increase rather than decrease these artificial oscillations. The examples in this contribution, however, clearly show the contrary. The main conclusion can therefore be summarised as follows:

High order finite element methods limit instead of increase the artificial oscillations in transport dominated problems. The solution converges exponentially to the exact solution when the polynomial degree of the Ansatz is increased.

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