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Jacobi galerkin spectral method for cylindrical and spherical geometries

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Abstract

The approximation of the convection–diffusion problem based on the Galerkin method in Cartesian, cylindrical and spherical coordinates is considered with emphasis in the last two cases. In particular, cylindrical and spherical coordinates can lead to a degeneracy in the global system of equations. This difficulty is removed by incorporating the factor r into the weight function which is introduced naturally by using Jacobi polynomials $P_k^{(\alpha,\beta)}$ with $\alpha=0$ and $\beta=1, 2$. By doing this, an unified framework is obtained for handling the typical geometries required in chemical engineering. Examples are presented based on the Galerkin method for discussing the applicability of this approach.

Keywords: Jacobi polynomials; Galerkin spectral methods; Convection–diffusion

1. Introduction

Typical geometrical configurations required in chemical engineering problems are the slab, cylinder and the sphere. For example, tubular reactors are normally described using 2D models with variations in (z, r) coordinates directions and catalyst used in industry are normally of cylindrical or spherical shape. The catalyst pellets are usually considered spherical and symmetric, reducing the spatial dimensionality to 1.

The classical reactor models consist of a set of species mass balances combined with a heat balance expressed in terms of temperature, as outlined in textbooks like Froment and Bishoff (1990) and Fogler (2006). Thus, this type of problems requires that a set of elliptic equation is solved. The equations are generally solved using finite difference (FDM), finite volume (FVM) or orthogonal collocation methods. In spite of this, the numerical solution of convection–diffusion problems constitute still an active area of research (Stynes, 2005). In particular, reactive systems are specially challenging due to the different temporal and spatial scales involved and because most real flows involve from few to hundreds of species, requiring in this way that a large number of coupled equations are solved. Spectral methods have shown to posses a relevant efficiency for complex problems such as supersonic reactive flows (Don and Gottlieb, 1998; Don et al., 2003) as compared to the other methods.

For convenience, differential equations can be rewritten in spherical or cylindrical coordinates. However, the transformations introduces a coordinate singularity at the origin in the case of cylindrical coordinates and at the origin and the pole in the spherical case. Some of the equations generate trivial algebraic relations $(0 = 0)$ resulting in an undetermined system of equations. The solution of the slab geometry by using spectral methods have been shown to produce optimal results, whereas for cylindrical and spherical geometries the convergence properties of the method can be severely affected.

For many singular problems, spectral methods can produce convergent solutions even with no special treatment. However, the singularities may be responsible for the very slow convergence degrading the accuracy or computational efficiency. The convergence can be accelerated significantly by imposing additional boundary conditions called *pole conditions* to capture the behavior of the solution as $r \to 0$ (Eisen et al., 1991; Huang and Sloan, 1993; Shen, 1997). A different approach is the use of Gauss Radau collocation nodes which exclude the center $r = 0$ avoiding the singularity there and therefore not

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requiring a pole condition (Chen et al., 2000). In order to avoid the singularity, Lai and Wang (2002) adopted a special Fourier series expansion together with grid shifting to nullify the numerical difficulties introduced by the singularity at the origin. On the other hand, Gerritsma and Phillips (2000) proposed to construct Jacobi polynomials incorporating the factor r into the weight function for axisymmetric problems.

In this work, the idea proposed by Gerritsma and Phillips (2000) is followed in order to avoid the singularities in the simulation of the convection–diffusion equation in cylindrical and spherical coordinates. The Lagrangian interpolant polynomial and quadrature rules are constructed in terms of Jacobi polynomials defined with a weight function which can compensate the singularity of the pole. The main relevance of applying the Jacobi polynomials is that a unified framework is obtained for handling the typical geometries required in chemical engineering.

In Section 2, a general convection–diffusion problem and its weak formulation (Deville et al., 2002) are presented for the three different coordinate systems. Section 3 describes the Jacobi polynomial in general and discusses how to construct basis function able to handle the different types of singularities. In Section 5, some numerical examples are discussed. Finally, Section 6 presents the main conclusions drawn from this work.

2. Convection–diffusion equation

A generic convection–diffusion problem can be written in cartesian, cylindrical and spherical coordinates as

$$\mathscr{L}u := -\frac{1}{\chi}\frac{\mathrm{d}}{\mathrm{d}r}\left[\chi\kappa\frac{\mathrm{d}u}{\mathrm{d}r}\right] + C\frac{\mathrm{d}u}{\mathrm{d}r} = g \quad \text{in } \Omega = (0, R), \tag{1}$$

$$\left.\frac{\mathrm{d}u}{\mathrm{d}r}\right|_{r=0} = 0, \tag{2}$$

$$u(R) = 0 \tag{3}$$

with $u \equiv u(r)$ the unknown function, $g \equiv g(r)$ a given source term, $\kappa \equiv \kappa(r)$ the diffusivity coefficient, $C \equiv C(r) > 0$ the velocity field and

$$\chi \equiv \chi(r) = \begin{cases} 1 & \text{cartesian coordinates,} \\ r & \text{cylindrical coordinates,} \\ r^2 & \text{spherical coordinates} \end{cases} \tag{4}$$

a function used for distinguishing the different coordinates systems.

The Galerkin formulation can be recasted in the equivalent weak form: find $u \in X(\Omega)$ such that

$$\mathscr{A}(u, v) = \mathscr{F}(v) \quad \forall v \in H_0^1(\Omega) \tag{5}$$

with the trial space defined as $X(\Omega) = \{u \mid u \in H^1(\Omega),\ u(R) = 0\}$ and

$$\mathscr{A}(u, v) := \int_0^R \left(\chi\kappa\frac{\mathrm{d}u}{\mathrm{d}r}\frac{\mathrm{d}v}{\mathrm{d}r} + \chi C\frac{\mathrm{d}u}{\mathrm{d}r}v\right)\mathrm{d}r, \quad v \in H_0^1(\Omega), \tag{6}$$

$$\mathscr{F}(v) := \int_0^R \chi g v\,\mathrm{d}r + \underbrace{\left[\chi\kappa v\frac{\mathrm{d}u}{\mathrm{d}r}\right]_{r=R}}_{=0}, \quad v \in H_0^1(\Omega), \tag{7}$$

where $H_0^1(\Omega)$ is the Sobolev space. The discretization of Eq. (5) consists in choosing a finite dimensional trial and test space, $X_N \subset X(\Omega)$. For convenience, it is considered that $X_N := \mathbb{P}_N \cap X(\Omega)$, with $\mathbb{P}_N$ the space of polynomials of degree less than or equal to N. Normally, the basis functions ϕ_i are chosen to be the set of Lagrangian interpolants on the GLL grid points r_q, i.e. $\phi_i(r_q) = \delta_{iq}$. The integral associated with the inner product in Eqs. (6) and (7) can be replaced by numerical quadrature with the quadrature points coinciding with the ones used for constructing the Lagrangian interpolant polynomials $\phi_i(r)$.

The discrete solution can be written as

$$u(r) = \sum_{j=0}^{N-1} u_j\phi_j(r). \tag{8}$$

By substituting expression (8) into Eq. (5), choosing systematically v to be ϕ_i and using quadrature integration, the resulting final algebraic equations can be written as

$$\begin{aligned}[\mathscr{A}]_{ij} &= \mathscr{A}_N(\phi_i, \phi_j) \\ &= \sum_{q=0}^{N} \omega_q\chi(r_q)\kappa(r_q)\phi_j'(r_q)\phi_i'(r_q) \\ &\quad + \sum_{q=0}^{N} \omega_q\chi(r_q)C(r_q)\phi_j'(r_q)\phi_i(r_q),\end{aligned} \tag{9}$$

$$[\mathscr{F}]_i = \mathscr{F}_N(\phi_i) = \sum_{q=0}^{N} \omega_q\chi(r_q)g(r_q)\phi_i(r_q), \tag{10}$$

where the evaluation of the integrals was performed by using Gauss integration, with r_q and ω_q the integration points and quadrature weights, respectively.

Letting $r \to 0$, then $\chi(r) \to 0$ for cylindrical and spherical coordinates, the first algebraic equation gives

$$[\mathscr{A}]_{0j} = \sum_{q=1}^{N} \omega_q\chi(r_q)\kappa(r_q)\phi_j'(r_q)\phi_0'(r_q) + 0, \tag{11}$$

$$[\mathscr{F}]_0 = 0 + 0. \tag{12}$$

In general, for all i, the first equation does not result in a $0 = 0$, as a consequence that integration by parts was used to transfer the derivative to the test function. However, the contribution of the convective operator to the algebraic system is zero, affecting the convergence property of the method.