On the Computation of Spectra of Spatially Varying Convective-Diffusion Operators

By

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Numerous applications in chemical engineering involve linear problems with spatially varying transport coefficients whose solutions can be obtained by spectral methods using the eigenvalues and eigenvectors of the associated Sturm-Liouville operators. Accurate computation of the spectra of Sturm-Liouville operators with non-constant coefficients require accurate numerical methods. In this connection, we demonstrate in this work, the effectiveness of the so-called Prufer transformation with respect to both computational speed and accuracy in comparison with Matlab methodology.

Motivation

Spatially varying problems arise naturally in turbulent transport. Consider, for example, the break-up of liquid droplets in turbulent flow of a continuous phase in which the droplets are immiscible. Assuming axisymmetry, variations occur in quantities of interest along the radial and axial directions. The population balance equation in the number density of drops in the i th size range, denoted $N_i(r,z)$ satisfies the following equation

$$Peu_z(r)\frac{\partial N_i(r,z)}{\partial z}-\frac{1}{r}\frac{\partial}{\partial r}\left(r\mathcal{D}(r)\frac{\partial N_i(r,z)}{\partial r}\right)$$
$$=\beta\Gamma_R(r)\left[-\Gamma_X^{(i)}N_i(r,z)+\sum_{k=i}^{n}\gamma_{i,k}\Gamma_X^{(k)}N_k(r,z)\right],\quad i=1,2,\ldots,n \qquad (1)$$

The details of the formulation are available in Ramkrishna and Nere (2007). The foregoing equation may be rewritten in more compact vector form as

$$Peu_z(r)\frac{\partial \mathbf{N}(r,z)}{\partial z}-\frac{1}{r}\frac{\partial}{\partial r}\left(r\mathcal{D}(r)\frac{\partial \mathbf{N}(r,z)}{\partial r}\right)=\beta\Gamma_R(r)\mathbf{A}\mathbf{N}(r,z) \qquad (2)$$

The boundary conditions may be written for $\mathbf{N}$ as

$$\frac{\partial \mathbf{N}}{\partial r}=\mathbf{0},$$

The solution of this problem can be readily obtained using the spectral decomposition of the Sturm-Liouville operator

The Sturm Liouville Operator

The Sturm-Liouville operator is given by

$$L\equiv-\frac{1}{w(x)}\frac{d}{dx}\left[p(x)\frac{d}{dx}\right]+q(x),\qquad a<x<b \qquad (3)$$

with homogeneous boundary conditions defining a domain $D(L)$ given by

$$u(a)\cos\alpha - p(a)u'(a)\sin\alpha = 0\,, \qquad u(b)\cos\beta - p(b)u'(b)\sin\beta = 0 \qquad (4)$$

for which the operator $\mathbf{L} = \{L, D(L)\}$ is self-adjoint. In particular note that p, q, w depend on x and are positive. The eigenvalues and eigenvectors, obtained by solving $\mathbf{Lu} = \lambda\mathbf{u}$, can be used to solve boundary value problems involving the operator $\mathbf{L}$. The solution of the differential equation $Lu(x) = \lambda u(x)$ provides $\mathbf{u}(\lambda) \equiv \{u(x,\lambda)\}$. The eigenvalues are obtained by demanding that $\mathbf{u}(\lambda) \in D(L)$. The problem of accurately determining the eigenvalues and eigenvectors can be difficult for the cases where p, q, w depend on x.

The Prufer Transformation

The Prufer transformation is as follows. Defining $u' = \frac{1}{p}v$, $v' = (q - \lambda w)u$, where primes denote differentiation with respect to x, we define polar coordinates, $v = r\cos\theta$, $u = r\sin\theta$. For nontrivial solutions, the differential equation $Lu = \lambda u$ leads to the pair of first order differential equations

$$\theta' = \frac{1}{p}\cos^2\theta + \lambda(w - q)\sin^2\theta, \quad \frac{r'}{r} = \left(\frac{1}{p} - \lambda w + q\right)\sin\theta\cos\theta \qquad (5)$$

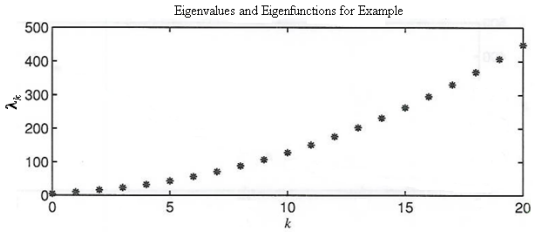
with boundary conditions $\theta(a) = \alpha, \quad \theta(b) = \beta$ obtained by transforming (4) . Since both boundary conditions involve only the function θ and the (nonlinear) differential equation for θ is independent of r, the differential equation in r may be integrated to obtain

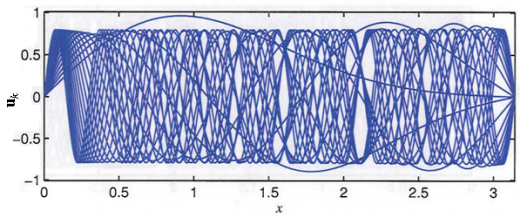
$$\ln|r(x)| = \int_{x_o}^{x}\left(\frac{1}{p(x')} - \lambda w(x') + q(x')\right)\sin\theta(x')\cos\theta(x')\,dx' \qquad (6)$$

where it is presumed that r does not vanish in the interval $a \le x \le b$. Since both boundary conditions are given in terms of only the function θ the calculation of eigenvalues involves only the integration of (5). The details concerning the calculation of the eigenvalues, available in a dissertation by Bohmann (2008), will be briefly included in the presentation. Broadly, however, the method involves the use of a shooting method to match the solution at some intermediate point c in the interval (a,b). Several academic examples were solved using the method, one of which is included in this abstract.

$$u'' + e^x u = \lambda u, \quad 0 < x < \pi; \qquad u(0) = u(\pi) = 0$$

The results of calculations are shown alongside for the eigenvalues and eigenvectors. The paper will discuss the methodology for solving the problem of drop break-up in fully developed flow of a liquid-liquid dispersion.





References

Bohmann, A., "Eigenvalue methods and the Prufer Transformation in Chemical Engineering," B.S. Thesis submitted to the University of Magdeburg and Purdue University, July 2008.