The following problem accompanies the book, Method of Weighted Residuals and Variational Principles, by Bruce A. Finlayson, a SIAM Classic reprinted in 2014. The original version was printed by Academic Press in 1972. See www.ChemEComp.com/MWR. Order the book from the Society of Industrial and Applied Mathematics, www.SIAM.org. The problems and solutions refer to equations and references in that book.

Problem 7 Solve the problem posed by a simplification of Eq. (11.176)

$$\nabla^2 u = f(u), \quad \frac{du}{dx}(0) = 0, \quad u(1) = 1, \text{ here } \frac{d^2u}{dx^2} = \phi^2 u, \quad \frac{du}{dx}(0) = 0, \quad u(1) = 1$$

for reaction and diffusion in a catalyst pellet with *Sh*->∞. The variable u is the concentration, the reaction rate is first order, and ϕ^2 is the Thiele modulus, representing the ratio of the rate of reaction to the rate of diffusion, and the equation is written for plane geometry.

a. First derive the exact solution to the problem.

b. Then use Hermite cubic finite elements and find approximate solutions for $\phi = 1$. Find upper bounds on the mean-square error and point-wise error. Show how the error bounds decrease as the number of degrees of freedom in the approximation increases. The formula for the mean square error is Eq. (11.174):

$$\|u - u_n\| \le \frac{\|R_n\| \|L^{-1}\|}{1 - K\|L^{-1}\|} \qquad (11.174)$$

Since $f = \phi^2 u$ the Lipshitz constant, *K*, is ϕ^2. The Green's functions and mean-square Green's functions for planar and spherical regions are:

$$G(x,t) = \begin{cases} 1 - x, t \le x \\ 1 - t, t \ge x \end{cases} \text{ (planar) and } G(x,t) = \begin{cases} \frac{1}{x} - 1, t \le x \\ \frac{1}{t} - 1, t \ge x \end{cases}$$

$$\|L^{-1}\| \equiv \left\{ \int_0^1 \int_0^1 G^2(x,t) x^{a-1} dx\, t^{a-1} dt \right\}^{1/2} = 1/\sqrt{6} \text{ (planar, } a\text{=1) and } 1/\sqrt{90} \text{ (spherical, } a\text{=3)}$$

(See Ferguson, N. B. and Finlayson, B. A., "Error Bounds for Approximate Solutions to Nonlinear Ordinary Differential Equations," *AIChE J.* **18** 1053-1059, 1972; see also http://faculty.washington.edu/finlayso/papers.html). They also prove that when the exact and approximate solution satisfy $0 \le u, u_n \le 1$ then

$$\|u-u_n\|_\infty \le K_2\left[K\|u-u_n\|_2+\|R\|_2\right]$$

which gives

$$\|u-u_n\|_\infty \le \frac{K_2\|R\|_2}{1-K\|L^{-1}\|} \quad \text{and} \quad \|u-u_n\|_\infty \le \frac{K_2\|R\|_2}{1-KK_1}$$

The constants are

$$K_1 = \max_{0\le x\le 1}\int_0^1 G(x,t)t^{a-1}dt = \frac{1}{2}(\text{planar}) \text{ or } \frac{1}{6}(\text{spherical})$$

$$K_2^2 = \max_{0\le x\le 1}\int_0^1 G^2(x,t)t^{a-1}dt = \frac{1}{3}(\text{planar}) \text{ or } \frac{1}{3}(\text{spherical})$$

These give slightly different results since

$$\|L^{-1}\| = 1/\sqrt{6} \text{ and } K_1 = 1/2 \text{ (planar) and } \|L^{-1}\| = 1/\sqrt{90} \text{ vs. } 1/6 \text{ (spherical)}$$

The error in the effectiveness factor is bounded by

$$|\eta-\eta_n| \le \frac{K\|u-u_n\|_\infty}{\left|f(u)|_{x=1}\right|}$$

c. Repeat with quadratic Lagrange quadratic finite elements.

d. Compare results from **b** and **c**.

Problem 8 Repeat Problem 7 for spherical geometry with Hermite cubic and Lagrange quadratic finite elements. To find the exact solution, make the substitution $z = u\, x$. Ferguson and Finlayson also prove that for a single equation, the Lipshitz constant K can be replaced by

$$\bar{K} = \sup_{0\le t\le 1}\left\{\int_0^1\left[\left.\frac{df(u)}{du}\right|_{u=c+t(c_n-c)}\right]^2 x^{a-1}\,dx\right\}^{1/2}$$

In this case exact solution and approximation are bounded below by 0 and above by 1.

Problem 9 Find approximate solutions to Problem 8 using a second-order reaction, $f(u)=\phi^2 u^2$. See Table 11.5. Use both Hermite cubic and Lagrange quadratic finite elements for $\phi = 1$ and 2.