The Reformulation and Numerical Solution of Certain Nonclassical Initial/Boundary Value Problems

Graeme Fairweather

Executive Editor Emeritus
Mathematical Reviews
American Mathematical Society
Ann Arbor, Michigan 48103, USA

In a Nutshell...

- (Initial-)Boundary Value Problems (IBVPs) arising in various applications are frequently not in the form required by existing general purpose software packages.
- However, **many problems can be easily converted** to such a form.
- We describe the conversion to “standard” form of some quite common “nonstandard” problems encountered in applications.

Déjà vu – all over again???

RECALL:

U. M. Ascher and R .D. Russell, “Reformulation of boundary value problems into ‘standard’ form”, SIAM Review 23 (1981) 238-254.

U. M. Ascher, R. M. Mattheij and R. D. Russell, ‘Numerical Solution of Boundary Value Problems for Ordinary Differential Equations”, Prentice Hall, NJ, 1988. Section 11.1.

Standard form required by several software packages

A first order system:

$$\mathbf{u}' = \mathbf{f}(x, \mathbf{u}), \quad x \in I \equiv (0, 1),$$
$$\mathbf{g}\left(\mathbf{u}(0), \mathbf{u}(1)\right) = \mathbf{0},$$

where **f** and **g** may be nonlinear.

- The boundary conditions could be **nonseparated** - for example, **periodic**: that is, $\mathbf{u}(0) = \mathbf{u}(1)$.
- Some packages can handle **mixed order systems** directly, but do not accept **nonseparated boundary conditions.**

Reformulation of Nonseparated Boundary Conditions

Recall:

$$\mathbf{g}\left(\mathbf{u}(0), \mathbf{u}(1)\right) = \mathbf{0}.$$

Introduce the constant function $\mathbf{v}$ such that

$$\mathbf{v}(x) = \mathbf{u}(1), \quad x \in I.$$

Then

$$\mathbf{u}' = \mathbf{f}(x, \mathbf{u}), \quad x \in I,$$
$$\mathbf{v}' = \mathbf{0}, \quad x \in I,$$

subject to the **separated** boundary conditions:

$$\mathbf{g}\left(\mathbf{u}(0), \mathbf{v}(0)\right) = \mathbf{0}, \quad \mathbf{u}(\mathbf{1}) = \mathbf{v}(\mathbf{1}).$$

$$u'' + \frac{s}{x}u' = R(u), \quad x \in I,$$

subject to the boundary conditions

$$u'(0) = 0, \quad u(1) = 1.$$

where $s = 1, 2$ for cylindrical and spherical geometries, respectively.

Problem? - *The singular coefficient*.

However.... since $u'(0) = 0$, and $\lim_{x\to 0} \dfrac{u'(x)}{x} = u''(0)$, using l'Hospital's rule, the DE at $x = 0$ is replaced by

$$u'' = \frac{R(u)}{(1+s)}.$$

Determine: $u(0)$.

Continuation

Consider

$$u'' + \frac{s}{x}u' + \lambda e^u = 0, \quad x \in I,$$
$$u'(0) = 0, \quad u(1) = 0,$$

- models the steady–state temperature distribution in:

- a cylinder of unit radius when $s = 1$;
- a sphere of unit radius when $s = 2$

with heat generation according to the exponential law.

Determine $u(0)$.

- No solution for $\lambda > 1.7$ when $s = 1$, and for $\lambda > 3.0$ when $s = 2.$.
- For values of λ close to these values, the corresponding BVPs are difficult to solve directly. USE CONTINUATION.

Note: As described earlier, when $x = 0$,

$$u'' + \frac{\lambda e^u}{(1+s)} = 0.$$

The governing equations reduce to:

$$f''' + \frac{1}{3}(m+2)ff'' - \frac{1}{3}(2m+1)(f')^2 = 0, \quad x \in [0, \infty),$$

where m is a parameter, subject to the BCs,

$$f(0) = 0,\ f''(0) = -1,\ f'(\infty) = 0,$$

Determine $f'(0)$.

- Replace the boundary condition at infinity by $f'(L) = 0$.
- Transform the BVP to

$$f''' + \frac{1}{3}L(m+2)ff'' - \frac{1}{3}L(2m+1)(f')^2 = 0, \quad x \in [0, 1],$$
$$f(0) = 0,\ f''(0) = -L^2,\ f'(1) = 0,$$

- Use continuation with an increasing sequence of values of L until $f'(0)$ remains constant to the desired accuracy.

Squeezing Flow of a Viscous Fluid between Elliptic Plates

Consider

$$f''' + k = SF(g,f), \quad g''' + \beta k = SF(g,f), \quad \text{on} \quad I \equiv [0,1],$$

subject to the BCs:

$$f(0) = f''(0) = g(0) = g''(0) = 0,$$

$$f(1) + g(1) = 2, \quad f'(1) = g'(1) = 0,$$

- F – a prescribed function, β S – prescribed constants.

NOTE: DE is of order **six** but there are **seven** BCs. However, since k is an unknown constant, add

$$k' = 0.$$

An Integral Constraint

Consider the constraint

$$\int_0^1 G(u(s), s)\, ds = R,$$

where R is a given constant.

Define

$$w(x) = \int_0^x G(u(s), s)\, ds,$$

and replace the constraint with

$$w'(x) = G(u(x), x),$$

and the boundary conditions

$$w(0) = 0, \quad w(1) = R.$$

Example - Membrane Separation Processes

Consider

$$u'' + \frac{1}{x}u' + c_1 + c_2\left(1 - e^{-\varphi(x,k)}\right)[\psi(u,\varphi) - 1] + c_3\psi(u,\varphi)u = 0,$$

subject to

$$u'(0) = 0, \qquad u(1) = 0,$$
$$\int_0^1 x\psi(u,\varphi)\,dx = c_4\int_0^1 xu\,dx,$$

where $\varphi(x,k)$ and $\psi(u,\varphi)$ are given functions and $c_i,\ i = 1,\dots,4$, are prescribed constants.

Determine u and the constant k.

Reformulation

First write the constraint as

$$\int_0^1 xF(u,x,k)dx = 0,$$

and set

$$w(x) = \int_0^x F(u,x,k)dx.$$

Then add to the original BVP:

$$w' = xF(u,x,k),$$
$$w(0) = 0, \quad w(1) = 0,$$

and

$$k' = 0.$$

Moving on to problems involving partial differential equations.....

Non-local Problems: Vibration Problems

The wave equation:

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$$

- a first approximation in the study of transverse vibrations of a string.

A better model:

$$\frac{\partial^2 u}{\partial t^2} = \left(1 + \int_0^1 \left(\frac{\partial u}{\partial s}\right)^2 ds\right) \frac{\partial^2 u}{\partial x^2}$$

Reformulation

Set

$$\psi = \frac{\partial u}{\partial t}, \qquad \phi = \frac{\partial u}{\partial x},$$

Then

$$\frac{\partial \phi}{\partial t} = \frac{\partial \psi}{\partial x},$$

Now let

$$w(x,t) = 1 + \int_0^x [\phi(s,t)]^2 ds.$$

Then

$$\frac{\partial \psi}{\partial t} = w(1,t)\frac{\partial \phi}{\partial x},$$

$$\frac{\partial w}{\partial x} = \phi^2, \qquad w(0,t) = 1.$$

Extensible Beam Equation

$$\frac{\partial^2 u}{\partial t^2}+\alpha\frac{\partial^4 u}{\partial x^4}-\left\{\beta+k\int_0^L\left[\frac{\partial u}{\partial s}(s,t)\right]^2 ds\right\}\frac{\partial^2 u}{\partial x^2}+c(x,t,u)=f(x,t),$$

where α, β, k are constants with α and k positive.

Set

$$\psi=\frac{\partial u}{\partial t}, \qquad \phi=\frac{\partial^2 u}{\partial x^2},$$

... and proceed in a similar manner.

Evolution in Time of the Age Structure of a Population

A first-order hyperbolic IBVP with **nonlocal BCs**:

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= -m(x)u, \quad x \in [0, A], t \geq 0. \\ u(0,t) &= f(E(t))E(t), \quad t > 0, \\ u(x,0) &= u_0(x), \quad x \in [0, A], \end{aligned}$$

where

$$E(t) = \int_0^A b(s)u(s,t)ds.$$

- $u(x,t)$ - population density at time t with respect to age x
- A - maximum attainable age
- $m(x)$, $b(x)$ - age-specific mortality rate and fertility rate, resp.

$$\frac{du(t)}{dt} = -\int_0^c \alpha(s)T(s,t)ds, \quad t > 0,$$

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(b(x)\frac{\partial T}{\partial x}\right) - q(x)T + \eta(x)\sigma(u(t)), \quad x \in [0,c], t > 0,$$

subject to the initial conditions

$$u(0) = u_0, \quad T(x,0) = f(x), \quad x \in [0,c],$$

and the boundary conditions

$$d_1 T(0,t) + d_2\frac{\partial T}{\partial x}(0,t) = 0, \quad t > 0,$$

$$d_3 T(c,t) + d_4\frac{\partial T}{\partial x}(c,t) = 0, \quad t > 0,$$

where

$$|d_1| + d_2| > 0, \qquad |d_3| + d_4| > 0,$$

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{1}{x}\int_a^b \rho \frac{\partial u}{\partial t}(\rho, t)\, d\rho, \quad (x, t) \in [a, b] \times [0, T],$$

subject to the boundary conditions

$$u(a, t) = f(t), \quad \frac{\partial u}{\partial x}(b, t) = g(t), \quad t \in (0, T],$$

and the initial condition

$$u(x, 0) = \phi(x), \quad x \in [a, b].$$

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad (x,t) \in I \times J,$$

$$u(x,0) = f(x), \quad x \in I, \qquad \frac{\partial u}{\partial x}(1,t) = g(t), \quad t \in J,$$

$$\int_a^b u(s,t)ds = F(t), \quad b \in I, \quad t \in (0,T],$$

where $I = (0,1), J \in (0,T]$, b is a given constant and f, g, F are prescribed functions

Define

$$w(x,t) = \int_0^x u(s,t)ds,$$

so that

$$\frac{\partial w}{\partial x}(x,t) = u,$$

$$w(0,t) = 0, \quad w(b,t) = \int_0^b u(s,t)ds = F(t).$$

Write the IBVP as a first order system: Let

$$v = \frac{\partial u}{\partial x}.$$

Then the differential equation becomes

$$\frac{\partial u}{\partial t} = \frac{\partial v}{\partial x},$$

and

$$u(x, 0) = f(x), \quad v(x, 0) = f'(x), \quad x \in I.$$

Also,

$$v(1, t) = g(t).$$

The IBVP

Thus:

$$\frac{\partial u}{\partial x} = v, \qquad \frac{\partial v}{\partial x} = \frac{\partial u}{\partial t}, \qquad \frac{\partial w}{\partial x} = u.$$

Let

$$I_h : 0 = x_0 < x_1 < \ldots < x_N = 1,$$

– a partition of $\bar{I} = [0, 1]$ with $h_i = x_i - x_{i-1}, \quad I = 1, \ldots N$.

Let

$$J_k : 0 = t_0 < t_1 < \ldots < t_M = T,$$

– a partition of the interval $[0, T]$ with $k_m = t_m - t_{m-1}, \ldots, M$.

Difference Operators

For a function $\Psi_{i,m}$ on the grid $\overline{I}_h \times J_k$, define on each cell $[x_{i-1}, x_i] \times [t_{m-1}, t_m]$,

$$\partial_x \Psi_{i,m} = \frac{\Psi_{i,m} - \Psi_{i-1,m}}{h_i}, \qquad \partial \Psi_{i,m} = \frac{\Psi_{i,m} - \Psi_{i,m-1}}{k_m}$$

$$\Psi_{i-1/2,m} = \frac{\Psi_{i,m} + \Psi_{i-1,m}}{2}, \qquad \Psi_{i,m-1/2} = \frac{\Psi_{i,m} + \Psi_{i,m-1}}{2}.$$

Let

$$U_{i,m} \approx u(x_i, t_m), V_{i,m} \approx v(x_i, t_m), \quad i = 0, \ldots, N, \quad m = 0, \ldots, M.$$

Suppose $b = x_K$, where K is an integer such that $0 < K \leq N$. Then

$$W_{i,m} \approx w(x_i, t_m), \quad i = 0, \ldots, K, \quad m = 1, \ldots, M.$$

Keller's Box Scheme

On each cell $[x_{i-1}] \times [t_{m-1}, t_m]$ of the grid $[I_h \times J_k]$, for $m = 1, \ldots, M$,

$$\begin{aligned}
\partial_x U_{i,m} &= V_{i-1/2,m}, \quad i = 1, \ldots, N, \\
\partial_x V_{i,m-1/2} &= \partial_t U_{i-1/2,m}, \quad i = 1, \ldots, N, \\
\partial_x W_{i,m} &= U_{i-1/2,m}, \quad i = 1, \ldots, K,
\end{aligned}$$

with the initial conditions:

$$\begin{aligned}
U_{i,0} &= f'(x), i = 0, \ldots, N-1, \\
V_{i,0} &= f'(x), i = 0, \ldots, N-1, \\
W_{i,0} &= 0, i = 0, \ldots, K-1,
\end{aligned}$$

and boundary conditions:

$$W_{0,m} = 0, \quad W_{K,m} = F(t_m), \quad V_{N,m} = g(t_m), \quad m = 1, \ldots, M.$$

Structure of the Coefficient Matrix

$$\begin{pmatrix} B & & & & & & & & \\ L_1 & R_1 & & & & & & & \\ & L_2 & R_2 & & & & & & \\ & & \ddots & \ddots & & & & & \\ & & & L_K & R_K & & & & \\ & & & & L_{K+1} & R_{K+1} & & & \\ & & & & & & \ddots & & \\ & & & & & & & L_N & R_N \\ & & & & & & & & C \end{pmatrix},$$

with

$$B = [0\ 0\ 1], \quad C = [0\ 1], \quad L_i = -I + \hat{L}_i, \quad i = 1, \ldots, N.$$

The matrix is **Almost Block Bidiagonal - ABB.**

For $1, \ldots, K$,

$$\hat{L}_i = \begin{bmatrix} 0 & -\frac{h_i}{2} & 0 \\ -\frac{h_i}{k_m} & 0 & 0 \\ -\frac{h_i}{2} & 0 & 0 \end{bmatrix}$$

and for $i = K+1, \ldots, N$,,

$$\hat{L}_i = \begin{bmatrix} 0 & -\frac{h_i}{2} \\ -\frac{h_i}{k_m} & 0 \end{bmatrix}$$

Also,

$$R_i = \hat{L}_i, \quad i = 1, \ldots, K-1, K+1, \ldots, N,$$

and

$$R_K = \begin{bmatrix} 0 & -\frac{h_K}{2} \\ -\frac{h_K}{k_m} & 1 \\ -\frac{h_K}{2} & 0 \end{bmatrix}$$

Alternate Row and Column Elimination

Alternate....

- **Row elimination with row pivoting**
  -partial pivoting with row interchanges followed by elimination by rows
  - *the standard procedure in Gaussian elimination*

with

- **Column elimination with column pivoting**
  - partial pivoting by columns with column interchanges, followed by elimination by columns

switching from one to the other when fill-in would occur otherwise

Key Reference

F. Majaess, P. Keast, G. Fairweather and K. R. Bennett, *Algorithm 704: ABDPACK and ABBPACK – FORTRAN programs for the solution of almost block diagonal linear systems arising in spline collocation at Gaussian points with monomial basis functions*, ACM Trans. Math. Software, 18 (1992), 205–210.

These codes can handle ABB systems in which the block matrix entries are not all the same size.

This example of Keller's Box Scheme is the ONLY example known to the developers which requires this feature.

A Much Studied Problem - Nonlocal Boundary Conditions.

Consider the heat equation

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f(x,t), \quad x \in [0,1], \quad t \in [0,T]$$

subject to the initial condition

$$u(x,0) = g(x), \quad x \in [0,1]$$

and the nonlocal boundary conditions:

$$u(0,t) = \int_0^1 \alpha(x)u(x,t)dx + g_0(t), \quad u(1,t) = \int_0^1 \beta(x)u(x,t)dx + g_1(t)$$

where $t \in [0,T]$ and α, β are given smooth functions.
Discretize the PDE using your favorite method with compatible quadrature approximations to the nonlocal conditions.

Example: Algebraic Problem

Structure of coefficient matrix at each time step.

$$A = \begin{bmatrix} x & x & x & x & x & x & x & x & x \\ x & x & x & & & & & & \\ & x & x & x & & & & & \\ & & x & x & x & & & & \\ & & & x & x & x & & & \\ & & & & x & x & x & & \\ & & & & & x & x & x & \\ & & & & & & x & x & x \\ x & x & x & x & x & x & x & x & x \end{bmatrix}$$

Capacitance Matrix Mathod

Let B be the matrix whose rows are the same as those of A except for the first and the last which are

$$[1, 0, \ldots, 0], \quad [0, \ldots, 0, 1]$$

corresponding to **Dirichlet boundary conditions.**

Let

$$\mathbf{c} = \mathbf{r} + \gamma_1 \mathbf{p} + \gamma_2 \mathbf{q}$$

where the numbers γ_1, γ_2 are to be determined and

$$B\mathbf{r} = [0, d_1, \ldots, d_n, 0]^T, \quad B\mathbf{p} = [1, 0, \ldots, 0, 0]^T, \quad B\mathbf{q} = [0, 0, \ldots, 0, 1]^T$$

Denote rows i of A and B by $A(i,\cdot)$ and $B(i,\cdot)$, respectively. Then since

$$A(i,\cdot) = B(i,\cdot), \quad i = 1,\ldots,N,$$

it follows that

$$A(i,\cdot)[\mathbf{r} + \gamma_1 \mathbf{p} + \gamma_2 \mathbf{q}] = d_i, \quad i = 1,\ldots,N.$$

Moreover,

$$A(i,\cdot)[\mathbf{r}+\gamma_1\mathbf{p}+\gamma_2\mathbf{q}] = A(i,\cdot)\mathbf{r}+\gamma_1 A(i,\cdot)\mathbf{p}+\gamma_2 A(i,\cdot)\mathbf{q}], \quad i = 0, N+!.$$

Determine γ_1, γ_2 from

$$\begin{bmatrix} A(0,\cdot)\mathbf{p} & A(0,\cdot)\mathbf{q} \\ A(N+1,\cdot)\mathbf{p} & A(N+1,\cdot)\mathbf{q} \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} d_0 \\ d_{N+1} \end{bmatrix}$$

References

- B. Bialecki, G. Fairweather and J. C. López-Marcos, The Crank-Nicolson Hermite cubic orthogonal spline collocation method for the heat equation with nonlocal boundary conditions, Adv. Appl. Math. Mech., 5(2013), 442–460.
- B. Bialecki, G. Fairweather and J. C. López-Marcos, The extrapolated Crank-Nicolson orthogonal spline collocation method for a quasilinear parabolic problem with nonlocal boundary conditions, J. Sci. Comput., 62(2015), 265–283.

A Parabolic Problem with Dynamic(al) Boundary Conditions

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \nabla.(a\nabla u), \quad (x,t) \in \Omega \times (0,T], \\
u(x,0) &= u_0(x), \quad x \in \Omega, \\
V\frac{\partial u}{\partial t} &= -a\frac{\partial u}{\partial \nu}, \quad (x,t) \in \partial\Omega \times (0,T],
\end{aligned}$$

- Ω - a bounded domain in R^n with smooth boundary $\partial\Omega$;
- $\frac{\partial}{\partial \nu}$ - outward normal differentiation;
- V - a positive constant.

Problems involving diffusion of solute into a solid from a well-stirred solution of fixed volume, V.

Examples:

- Diffusion of dye into a fiber from a finite dye-bath. **(Crank)**
- Heat conduction when the surface of a solid is in perfect thermal contact with a well-stirred fluid (or a perfect conductor). **(Carslaw & Jaeger)**
- Leeching of nitrogen from the soil by floodwaters in the Mississippi River Delta.

The Weak Form

Suppose $v \in H^1(\Omega)$. Then

$$\left(\frac{\partial u}{\partial t}, v\right) + (a\nabla u, \nabla v) + < a\frac{\partial u}{\partial \nu}, v >= 0,$$

or

$$\begin{aligned}\left(\frac{\partial u}{\partial t}, v\right) + (a\nabla u, v) + < \frac{\partial u}{\partial t}, v > &= 0, \quad v \in H^1(\Omega), \quad t \in (0, T], \\ u(x, 0) &= u_0(x), \quad x \in \Omega.\end{aligned}$$

QuiteEasilyDone

An Overlooked Paper....

G. Fairweather, *The approximate solution of a diffusion problem by Galerkin methods*, J. Inst. Maths. Applics., 24 (1979), 121-137.

NO WONDER!!

Its title gives no indication of the nature of the problem.

A New Title...

The approximate solution of a diffusion problem

with dynamic(al) boundary conditions

by Galerkin methods.

In MathSciNet:

– 35 papers with “Dynamic boundary conditions” - since 2008.

- 8 with “Dynamical boundary conditions”.

In the future...

- Analysis of Keller's method - *an ongoing struggle*.
- A survey article on non-local problems.

THANK YOU

FOR

YOUR ATTENTION