NUMERICAL METHODS FOR BOUNDARY VALUE PROBLEMS WITH APPLICATION TO BIFURCATION PROBLEMS

Eusebius Doedel

Department of Computer Science, Concordia University, Montreal, Canada

Abstract *The method of orthogonal collocation for solving boundary value problems in ordinary differential equation is described, and its relationship to classical finite difference methods is illustrated. Numerical examples demonstrate the capabilities of software based on orthogonal collocation for analyzing nonlinear differential equations. A new discretization method for the solution of elliptic partial differential equations is described. It is indicated how this method can also be viewed as a collocation method. Numerical results illustrate its accuracy.*

Collocation and Finite Differences. Consider the following boundary value problem (BVP) for the ordinary differential equation (ODE)

$$u''(t) \ + \ a(t)\, u'(t) \ + \ b(t)\, u(t) \ = \ f(t), \qquad t \in [0,1],$$

$$u(0) \ = \ u(1) \ = \ 0.$$

Assume that the coefficient functions and the inhomogeneous term are sufficiently smooth and that the corresponding homogeneous problem only admits the zero solution. Our main interest is nonlinear ODE BVPs, but to keep the presentation simple, we describe numerical methods only for linear equations.

Introduce a *mesh* $0 = t_0 < t_1 < t_2 < \cdots < t_N = 1$, with $h_j \equiv t_j - t_{j-1}$ and $h \equiv \max_j t_j$. The method of *orthogonal collocation with piecewise polynomials* consists of finding $p \in C^1[0,1]$ such that p is a polynomial of degree $\leq m+1$ in each mesh interval $[t_{j-1}, t_j]$, $(j = 1, 2, \cdots, N)$, and such that p satisfies the *collocation equations*

$$p''(z_{ji}) \ + \ a(z_{ji})\, p'(z_{ji}) \ + \ b(z_{ji})\, p(z_{ji}) \ = \ f(z_{ji}), \quad i = 1, \cdots, m, \quad j = 1, 2, \cdots, N,$$

and the boundary conditions

$$p(0) \ = \ p(1) \ = \ 0 \ .$$

Here the m *collocation points* z_{ji} $i = 1, \cdots, m$ lie in the jth mesh interval $[t_{j-1}, t_j]$ and are distinct, but otherwise arbitrary. It is easily checked that the number of equations is formally enough to determine p. A rigorous existence and convergence proof shows that the global accuracy of the approximate solution is given by

$$max_{[0,1]} \mid p(t) - u(t) \mid = \mathcal{O}(h^{m+1}).$$

However, if in each subinterval $[t_{j-1}, t_j]$ the m collocation points are chosen as the (scaled and translated) roots of the mth degree Legendre orthogonal polynomial, then we have *superconvergence* [1] at the main meshpoints t_j :

$$max_j \mid p(t_j) - u(t_j) \mid = \mathcal{O}(h^{2m}).$$

In practice, the choice $m = 4$ is often used. In particular, this is the choice in the numerical examples presented below. Note that this gives 8th order accuracy at the mesh points. This means that, in an asymptotic sense, the error at the mesh points is reduced by a factor 2^8 by doubling the number of mesh intervals, i.e., for just twice the computational work. If the boundary value problem includes scalar unknowns, for example the period of a limit cycle in a dynamical system (see below), then these also have superconvergent accuracy.

In addition to simplicity and accuracy, the orthogonal collocation method also has the advantage of having a known optimal algorithm for placing the mesh points t_j (See [2,3]). These advantages make the method very suitable for solving difficult linear and nonlinear problems, as illustrated below.

Finite Difference methods are the earliest methods used to numerically solve ODE BVPs. The simplest finite difference method for solving our linear BVP consists of finding u_j, $(j = 0, \cdots, N)$, such that

$$\frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} \; + \; a(t_j)\,\frac{u_{j+1} - u_{j-1}}{2\,h} \; + \; b(t_j)\,u_j \;=\; f(t_j), \qquad j = 1, 2, \cdots, N-1.$$

with

$$u_0 \;=\; u_N \;=\; 0.$$

Actually, this finite difference method is equivalent to the collocation method illustrated in Figure 1. Each of the local polynomials p_j matches pointwise to its neighbors, as indicated. Furthermore, for each j, p_j is required to satisfy the differential equation at the mesh point t_j. In addition, the outermost polynomials must satisfy the boundary conditions.

This collocation interpretation of finite differences immediately suggests a generalization to non-uniform meshes. The most obvious generalization, with collocation at the mesh points t_j, is only first-order accurate. However, it is easily shown [4] that a second order method is obtained if, for each j, the collocation point is given by $(t_{j-1}+t_j+t_{j+1})/3$.

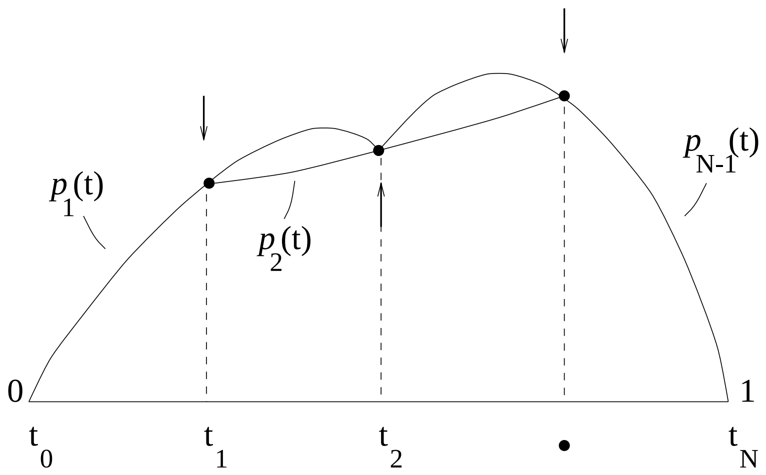

Figure 1: *Equivalent collocation method* ($p_j \in \mathbf{P}_2$).

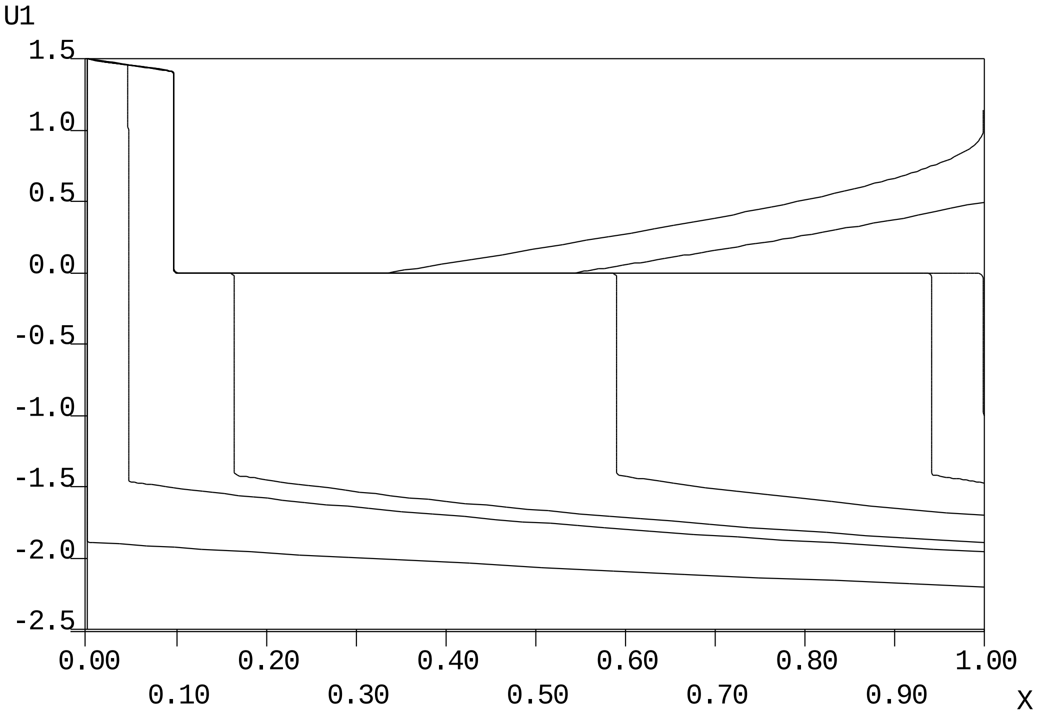

Figure 2: *BVP solutions for various γ; with $\epsilon = 10^{-5}$.*

Note that, for the orthogonal collocation method, we required the piecewise polynomials to be globally once continuously differentiable. Similarly, the collocation interpretation of finite differences uses multivalued piecewise polynomial spaces in which, by Rolle's Theorem, neigboring polynomial have matching derivatives at some point. Thus, in some sense, these multi-valued approximate solutions are also globally once continuously differentiable. Similarly, for kth order differential equations, the degree of continuity should, in some sense, be equal to $k-1$. For such a discretization convergence is guaranteed, even on nonuniform meshes, as the mesh size tends to zero [5,6].

Applications

Consider the singularly perturbed ODE BVP

$$\epsilon u'' \;-\; u\, u'\,(u^2-1) \;-\; u \;=\; 0,$$

with boundary conditions

$$u(0) \;=\; \frac{3}{2}, \qquad u(1) \;=\; \gamma.$$

This equation was studied in [7]. Varying γ gives rise to several qualitatively distinct solutions, as illustrated in Figure 2.

In calculations with the software AUTO [8], a *continuation* (or *homotopy*) method is used to sweep out the entire range of γ-values. This ensures that all solution types are located. The number of continuation steps is moderate when γ is not too small, for example, $\gamma = 10^{-3}$. However, for $\gamma = 10^{-5}$, as in Figure 2, the number of required continuations steps is very large, so that the calculation requires a lot of computer time. If γ is even smaller, say, $\gamma = 10^{-8}$, then the CPU time becomes prohibitive. Indeed, in such extreme cases, one may have to turn to classical perturbation techniques, or to corresponding specialized numerical techniques.

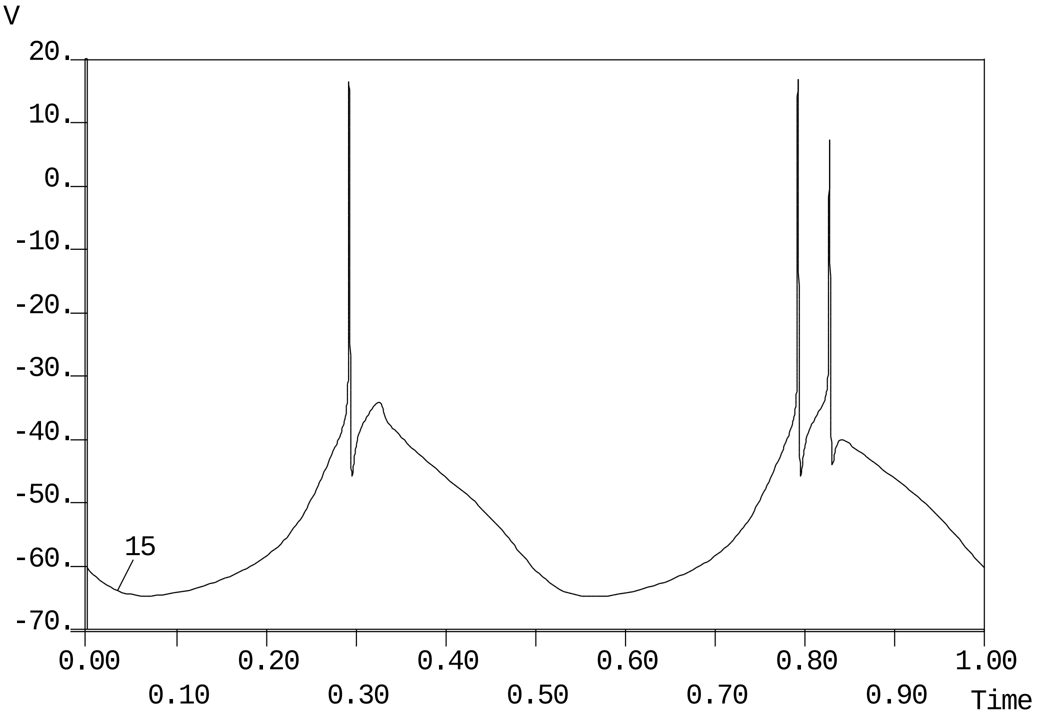

Figure 3: *A bursting solution (after period-doubling).*

As a second computational example consider periodic solutions to dynamical systems. In many applications it is important to determine periodic solutions. When these are asymptotically stable they can, in principle, be computed by time integration with suitable initial conditions. However, this may require a long integration time, especially near critical points, such as Hopf, period-doubling, and torus bifurcations. Asymptotically unstable periodic orbits can, in general. not be computed at all by numerical time integration. Such orbits are often essential in the understanding of the global dynamics of a system, or they may be stabilized and hence made physically important. For these reasons, we use a boundary value approach to compute period orbits. More precisely, a solution $(u(\cdot), T)$ of the boundary value problem

$$u'(t) = Tf(u(t), \lambda),$$
$$u(0) \;=\; u(1),$$

corresponds to a solution of period T of the dynamical system $u'(t) = f(u(t), \lambda)$. For uniqueness, a phase condition must to be added to the above BVP. See [8] for details.

As an application consider Plant's model of bursting nerve cells [9]. It has the form

$$\dot{V} = [g_I s_I^3(V) y_I + g_T x_T][V_I - V] \;+\; [g_K x_K^4 + g_P c(K_p + c)^{-1}][V_K - V] \;+\; g_L[V_L - V],$$

$$\dot{x}_T = [s_T(V) - x_T]/(\zeta \tau_{xT}),$$
$$\dot{x}_K = [s_K(V) - x_K]/(\zeta \tau_{xK}),$$
$$\dot{y}_I = [z_I(V) - y_I]/(\zeta \tau_{yI}),$$
$$\dot{c} = \rho[K_c x_T(V_{Ca} - V) - c],$$

for certain coefficient functions $s_I(V)$, $s_T(V)$, etc. A periodic solution computed by the BVP approach is shown in Figure 3. Actually, this solution results from a period-doubling bifurcation encountered in the continuation process. Numerical methods for dealing with such phenomena have been incorporated into software such as AUTO.

Another application of numerical BVP methods concerns *connecting orbits* in dynamical systems. These are important in the study of traveling wave fronts and pulses. Their numerical computation can be posed as BVP of the form

$$u'(t) \;=\; T\ f(u(t),\lambda), \qquad u(\cdot), f(\cdot,\cdot) \in \mathrm{R}^n, \quad \lambda \in \mathrm{R}^{n_\lambda},$$

with boundary conditions

$$B_0\ \Big(u(0) - w_0\Big) \;=\; 0, \qquad B_1\ \Big(u(1) - w_1\Big) \;=\; 0.$$

Here T is "large" and, typically, fixed. The above equations are to be solved for $u(t)$ and λ. B_0 and B_1 represent boundary conditions that require the solution $u(t)$ to approximately start and end in the unstable/stable manifold of rest points w_0, w_1, respectively. Other constraints, such as a phase condition, may also be imposed. For details see [10,11,12,13].

As a specific example consider a model of two coupled Josephson junctions [14,15] :

$$\beta\phi_j'' + \phi_j' + \sin\phi_j - \frac{3}{2(3+\beta)}\sum_{k=1}^{2}(\phi_k' + \sin\phi_k) = \frac{\beta}{3+\beta}I, \qquad (j = 1,2).$$

where ϕ_j is the phase difference across the gap in the j-th junction, β is the intrinsic capacitance of the individual junctions, and I is a bias current. These equation can be rewritten as a dynamical system in R^4. The projection of a numerically computed connecting orbit onto the (ϕ_1, ϕ_2)-plane is shown in Figure 4. This orbit has a large, but finite, period, and approximates a connecting orbit, whose period is infinite. Actually, a multitude of qualitatively distinct connecting orbits were found for this model. The numerical analysis shows that many of these arise from a specific "organizing center" in parameter space (β, I). These findings motivated the mathematical study in [16].

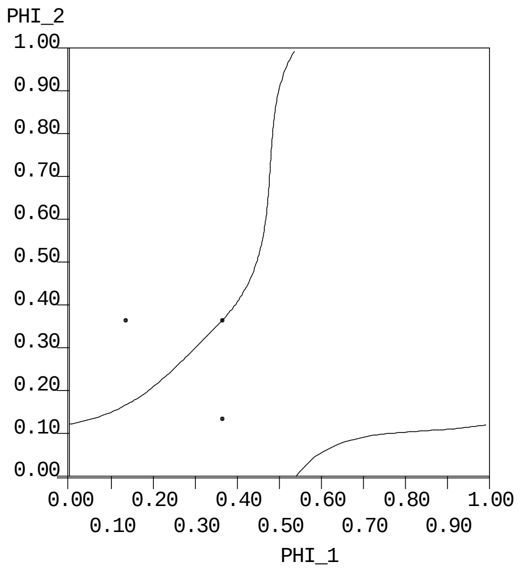

Figure 4: *A projected connecting orbit. The phases, ϕ_1 and ϕ_2, are scaled by 2π. Three rest points are indicated, including the one on the connecting orbit.*

New Collocation Methods for PDEs

Our main interest is the numerical analysis of bifurcation problems in nonlinear systems of elliptic partial differential equations (PDEs). However, to keep the presentation as simple as possible, we here consider the Laplace equation on a square :

$$\Delta u = f(x), \qquad x \in \Omega \subset \mathrm{R}^2,$$

$$u(x) = g(x), \qquad x \in \partial\Omega.$$

The square, Ω, has been recursively subdivided, as in Figure 5. The smallest elements of the subdivision are called "*finite elements*". Figure 6 shows a finite element, with n points x_i on its boundary and m points z_i in its interior.

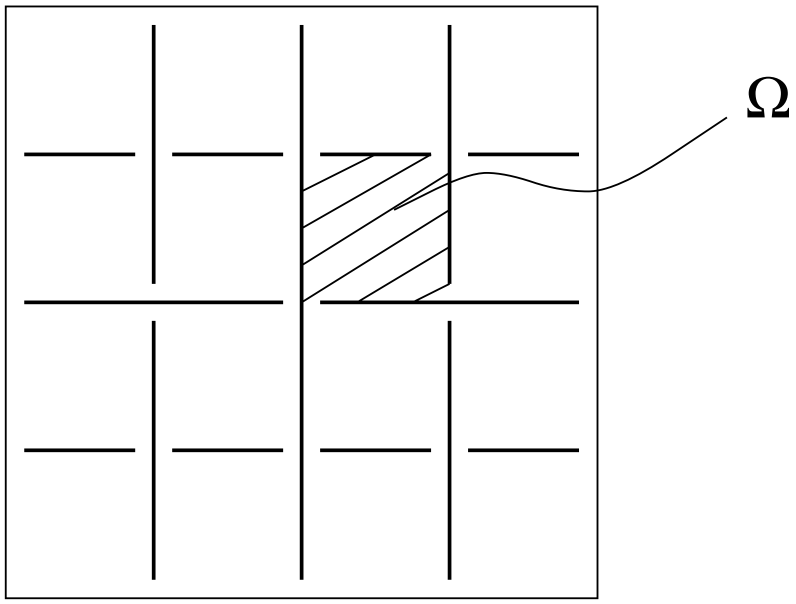

Figure 5: *The domain Ω and its recursive subdivision.*

The *finite difference* approach uses a formula of the form

$$v_i \;=\; \sum_{j=1}^{n} \alpha_{ij}\; u_j \;+\; \sum_{j=1}^{m} \beta_{ij}\; f(z_j),$$

corresponding to each point x_i on the element boundary, for each element. Here u_j and v_j represent the as yet unknown approximate solution and its derivative normal to the boundary, respectively. The above relation represent a discrete version of the following consequence of ellipticity: If an element is sufficiently small, and if the solution is given on the element boundary then the derivative of the solution normal to the boundary is uniquely determined at each boundary point. (Some smoothness is assumed here.)

For each i, the coefficients α_{ij} and β_{ij} can be determined by requiring that

$$\nabla\phi(x_i)^*\eta_i \;=\; \sum_{j=1}^{n} \alpha_{ij}\; \phi(x_j) \;+\; \sum_{j=1}^{m} \beta_{ij}\; \Delta\phi(z_j),$$

for all polynomials $\phi \in P_{n+m}$. Here P_{n+m} denotes an appropriate function space (typically polynomials) of dimension $n+m$. Above, η_i is the normal to the element boundary at x_i, and * denotes transpose.

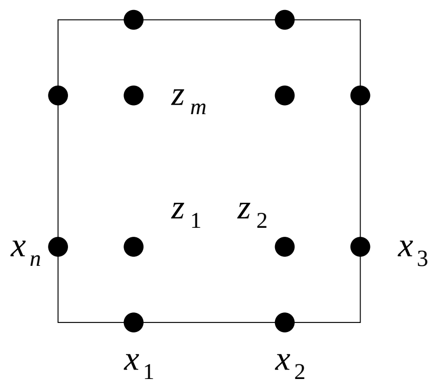

Figure 6: *A finite element of* Ω.

If we define $u = (u_1, \cdots, u_n)^*$, $v = (v_1, \cdots, v_n)^*$, $f = (f(z_1), \cdots, f(z_m))^*$, and

$$A = \begin{pmatrix} \alpha_{11} & \cdots & \alpha_{1n} \\ \vdots & & \vdots \\ \alpha_{n1} & \cdots & \alpha_{nn} \end{pmatrix}, \qquad B = \begin{pmatrix} \beta_{11} & \cdots & \beta_{1m} \\ \vdots & & \vdots \\ \beta_{n1} & \cdots & \beta_{nm} \end{pmatrix},$$

then the discrete equations can be written as

$$v \;=\; A\,u \;+\; B\,f.$$

Also define

$$\Phi = \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_1(x_n) \\ \vdots & & \vdots \\ \phi_{n+m}(x_1) & \cdots & \phi_{n+m}(x_n) \end{pmatrix}, \qquad \Delta_\Phi = \begin{pmatrix} \Delta\phi_1(z_1) & \cdots & \Delta\phi_1(z_m) \\ \vdots & & \vdots \\ \Delta\phi_{n+m}(z_1) & \cdots & \Delta\phi_{n+m}(z_m) \end{pmatrix},$$

$$\mathrm{R}_\Phi = \begin{pmatrix} \nabla\phi_1(x_1)^*\eta_1 & \cdots & \nabla\phi_1(x_n)^*\eta_n \\ \vdots & & \vdots \\ \nabla\phi_{n+m}(x_1)^*\eta_1 & \cdots & \nabla\phi_{n+m}(x_n)^*\eta_n \end{pmatrix},$$

where

$$Span\{\phi_1, \cdots, \phi_{n+m}\} = P_{n+m}.$$

Then the coefficients can be computed by solving

$$(\,\Phi \quad \Delta_\Phi\,)\begin{pmatrix} A^* \\ B^* \end{pmatrix} \;=\; R_\Phi.$$

For appropriate choice of the points x_i and z_i, the matrix $(\,\Phi \quad \Delta_\Phi\,)$ is indeed nonsingular. In such case the finite difference construction is well-defined.

The above finite difference method can be shown to be equivalent to the following collocation method: Associate a polynomial $p(x) \in P_{n+m}$ to each finite element. (Here and below we suppress indices denoting the element.) Require that at the points x_i on any common boundary the values of neigboring polynomials, as well as their normal derivatives, match. Further, require each polynomial to satisfy the *collocation* equations

$$\Delta p(z_k) = f(z_k) \qquad k = 1, \cdots, m.$$

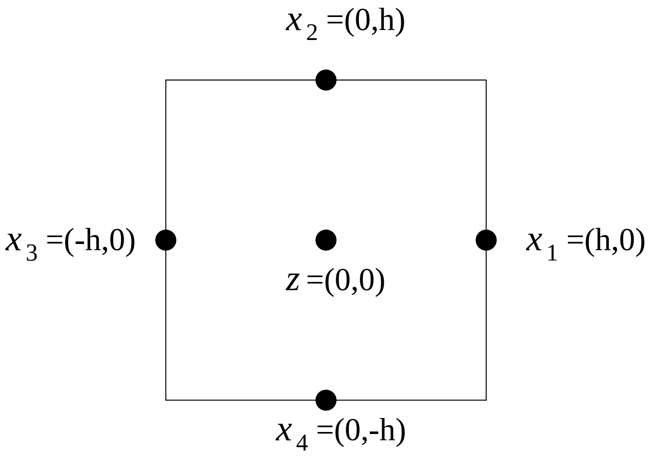

Figure 7: *Template for an element with $m = 1$, $n = 4$.*

As a simple example consider the case of one matching point per element boundary, and one collocation point per element, as in Figure 7. In this case the finite difference formulation has the form

$$v_i = \sum_{j=1}^{4} \alpha_{ij} u_j \ + \ \beta_i f(z).$$

As a basis of $P_{n+m} = P_5$ choose $\{1, x, y, x^2, y^2\}$. Then, for each finite element, the finite difference equations are found to be

$$\begin{aligned} v_1 &= (2u_1 - u_2 - u_4)/2h + hf(z)/2, \\ v_2 &= (2u_2 - u_1 - u_3)/2h + hf(z)/2, \\ v_3 &= (2u_3 - u_2 - u_4)/2h + hf(z)/2, \\ v_4 &= (2u_4 - u_1 - u_3)/2h + hf(z)/2. \end{aligned}$$

This method is second order accurate. Other choices of the matching and collocation points can give higher order accuracy, as illustrated in Table 1.

Nested dissection

The finite difference formulation lends itself very naturally to solution by *nested dissection*: Consider two adjacent finite elements Ω_1 and Ω_2, as in Figure 8. Using the combined finite difference equations for each of the two elements, one can eliminate the unknown u's and v's corresponding to common boundary $\partial\Omega_{12}$. This procedure can be repeated recursively, to finally lead to a similar set of equations for the boundary of the full square Ω. Using the boundary conditions, one can then compute the v's on the boundary of Ω. Finally, a backsubstitution yields the u's and v's in the interior of Ω.

The advantage of the nested dissection algorithm is its reduced computational complexity. For an M by M mesh, a dense matrix solver would take $O(M^6)$ operations. Of course, this is extremely inefficient. However, the more efficient "band-solver" still takes $O(M^4)$, while the nested dissection takes only $O(M^3)$.

To summarize, the PDE collocation method offers several advantages. High order accuracy is possible, as illustrated in Table 1. Furthermore, the nested dissection solution algorithm is relatively easy to implement, and can reduce computational cost. Nested dissection also offers certain advantages for bifurcation problems. Finally, it is conjectured that a subclass of the collocation methods has very good numerical stability properties, even on nonuniform meshes.

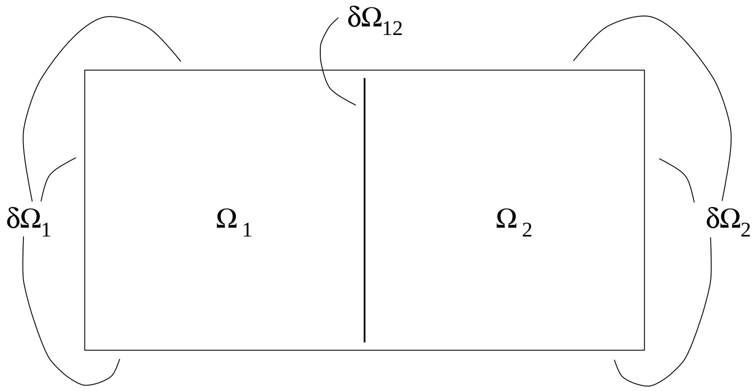

Figure 8: *Two adjacent elements (or regions).*

The above PDE collocation methods are described in more detail in [17]. For somewhat related work, see [18]. For "conventional" PDE collocation methods see, for example, [19,20].

h	$\kappa = 1$		$\kappa = 2$		$\kappa = 3$		$\kappa = 4$	
$\frac{1}{2}$	5.44^{-4}	(0.05)	6.87^{-6}	(0.10)	5.90^{-7}	(0.10)	6.47^{-9}	(0.20)
$\frac{1}{4}$	1.50^{-4}	(0.08)	3.26^{-7}	(0.14)	2.40^{-8}	(0.23)	1.45^{-10}	(0.34)
$\frac{1}{8}$	3.78^{-5}	(0.20)	1.48^{-8}	(0.40)	8.61^{-10}	(0.82)	2.76^{-12}	(1.4)
$\frac{1}{16}$	9.51^{-6}	(0.79)	7.67^{-10}	(1.8)	2.88^{-11}	(4.2)	4.65^{-14}	(7.5)

Table 1: *Maximum error at the matching points, and CPU time per Newton iteration, for a model problem on the unit square, for various mesh sizes h and various choices of κ. Each element has κ^2 collocation points and κ matching points per element boundary.*

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