A radically new method for solving boundary-layer problems illustrates the cross-disciplinary nature of basic research. The method, which is applicable to singular perturbation problems in many fields, was developed in the context of particle physics.

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by Carl M. Bender

LOS ALAMOS SCIENCE

P roblems involving a rapid change in the value of a physical variable over a limited region of space or time are common in physics. They are referred to as boundary-layer problems. The most familiar examples occur in the motion of fluids. In these cases, a boundary layer refers to the very narrow region of fluid moving along a solid surface or boundary such as the inside of a pipe or a river bed; the fluid velocity in the boundary layer varies rapidly from zero at the boundary to the free-stream velocity away from the boundary. The boundary layer becomes narrower as the viscosity η decreases. This kind of dependence on viscosity means that the differential equation describing the fluid exhibits singular

behavior and cannot be handled adequately by conventional perturbation methods when η is small.

Our new, very general approach to singular perturbation problems enables us to solve nonlinear and high-order boundary-layer problems without resorting to large-scale computer codes to study the systems mimetically. The central idea consists of replacing the differential equation for the problem by a discrete equation defined on a lattice. After solving the discrete problem using regular perturbation techniques, we invoke special techniques to recover the continuum answers in the limit as the lattice spacing vanishes.

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Perturbation Theory

Perturbation theory is a vast collection of mathematical methods used to obtain approximate solutions to problems that have no closed-form analytical solutions. The methods work by reducing a hard problem to an infinite sequence of relatively easy problems that can be solved analytically. Often, solving the first few of these provides an accurate approximation to the solution of the original hard problem.

A simple example illustrates the idea of perturbation theory. Consider the quintic polynomial

$$X^{5} + x - 1 = 0 . (1)$$

By drawing a graph of this equation and showing that its slope is always positive, we see that Eq. (1) has just one positive root. We cannot determine its numerical value analytically because there is no algebraic formula for the roots of a quintic polynomial. However, a perturbative approach reduces the problem to a sequence of almost trivial problems.

First, we introduce a perturbation parameter ε , which we specify to be small.

$$\mathbf{x}^5 + \mathbf{\varepsilon}\mathbf{x} - \mathbf{1} = \mathbf{0} \quad . \tag{2}$$

With ε small, we assume that the roots x(E) have a Taylor expansion in powers of ε .

$$\mathbf{x}(\mathbf{\varepsilon}) = \mathbf{a} + \mathbf{b}\mathbf{\varepsilon} + \mathbf{c}\mathbf{\varepsilon}^2 + \mathbf{d}\mathbf{\varepsilon}^3 + \dots$$
 (3)

Using this expansion we represent the terms in Eq. (2) as expansions:

$$\begin{aligned} x(\epsilon)^5 &= a^5 + 5a^4b\epsilon + (5ca^4 + 10a^3b^2)\epsilon^2 \\ &+ (5a^4d + 20a^3bc + 10a^2b^3)\epsilon^3 + ... \end{aligned}$$

and

$$\epsilon \mathbf{x}(\epsilon) = \mathbf{a}\epsilon + \mathbf{b}\epsilon^2 + \mathbf{c}\epsilon^3 + \dots$$

Substituting these expansions into Eq. (2), collecting the coefficients of like powers of E, and setting them equal to zero gives a sequence of equations that are easily solved for the coefficients of Eq. (3).

- $a^{\circ} 1 = 0 \rightarrow a = 1$ (here we take the real root),
- b^{1} : $5a^{4}b + a = 0 \rightarrow b = -1/5$,
- b^{2} ;²) $5ca^{4} + 10a^{3}b^{2} + b = 0 \rightarrow c = -1/25$,
- z^{3}) $5a^{4}d + 20a^{3}bc + 10a^{2}b^{3} + c = 0 \rightarrow d = -1/125$,

and so on. We thus have determined that

$$\kappa(\varepsilon) = 1 - \varepsilon/5 - \varepsilon^2/25 - \varepsilon^3/125 + \dots$$

The perturbation parameter ε plays a crucial role because it organizes the hard problem in Eq. (1) into a sequence of much easier problems, which in this case involve finding the coefficients a, b, c, d,

If we set & = 1, we recover the original Eq. (1) from Eq. (2) and obtain a rapidly convergent series representation for its perturbative solution.

$$\kappa(1) = 1 - \frac{1}{5} - \frac{1}{25} - \frac{1}{125} + \dots = 0.752 \quad . \tag{4}$$

The exact value for x(1) found by solving Eq. (1) numerically on a computer is 0.754878.... Thus, our perturbation solution is impressively accurate. We could have found perturbation series for the other four (complex) roots by starting with any of the other four solutions to $a^s - 1 = O$.

Singular Perturbation Problems

The problem just considered is a *regular* perturbation problem; that is, its solutions vary smoothly as the perturbation parameter ε approaches zero. The problems of interest here are *singular* perturbation problems; their solutions change abruptly in some way as ε reaches zero. Some or all solutions either might cease to exist or might become infinite or degenerate. To illustrate, we can make Eq. (1) into a singular perturbation problem by introducing E in a different way, for example,

$$\varepsilon x^{5} + x - 1 = 0 .$$

This problem is singular because E multiplies the highest power of x in the equation. As a result, when $\varepsilon \to 0$, the degree of the polynomial suddenly changes from 5 to 1. Moreover, a fifth-degree polynomial has five roots and a first-degree polynomial has one root, so in the limit $\varepsilon \to 0$ four roots disappear entirely. As $\varepsilon \to 0$, the roots move off to infinity in the complex plane according to $|x| \sim \varepsilon^{-1/4}$. (See Fig. 1.) The fact that the character of this problem changes abruptly as $\varepsilon \to 0$ identifies it as a singular perturbation problem.

The series expansions for singular perturbation problems are more complicated than the Taylor series in Eq. (3). Often they are not in Taylor form (a series in integer powers of ϵ_{J} , and usually they are divergent series. These problems sound so formidable that one might be tempted to avoid them completely. However, avoiding them is often not possible or even



Fig. 1. The dots indicate the position of the five roots $x(\varepsilon)$ of $\varepsilon x^{5} + x - 1 = 0$ as $\varepsilon \to 0$. One root approaches 1 while the other four move out to infinity according to $|x| \sim \varepsilon^{-1/4}$.

desirable. In many physical problems, a natural small parameter ϵ occurs in such a way that the problem is automatically singular. For example, the time-independent Schrodinger equation,

$$-\frac{h^2}{2m} \nabla^2 \psi(\vec{x}) + [V(\vec{x}) - E] \psi(\vec{x}) = 0 ,$$

contains the natural small parameter $h^2/(2m)$. In the classical limit of the quantum system defined by $h^2/2m \rightarrow 0$, this equation becomes a singular perturbation problem because its character changes abruptly from a differential equation to an algebraic equation.

Even when physics doesn't dictate that a perturbation problem be singular, we may want to introduce a perturbation parameter ε to make the problem singular. Although the resulting perturbation series may be divergent, it is usually asymptotic. (Roughly speaking, an asymptotic series $\Sigma a_n \varepsilon^n$ is one that diverges but also has the remarkable property that the first few terms provide an accurate approximation to the sum for sufficiently small ε .) Moreover, using modern summation techniques that have come into wider use over the last 20 years (Pade approximants and the Bore] summation), we may obtain a more accurate numerical result from 3 or 4 terms of the divergent series than from 10 or 20 terms of a convergent series even when the perturbation parameter ε is large.

Boundary-Layer Theory

Boundary-layer problems, a special class of singular perturbation problems, provide the simplest context for introduc-

Fig. 2. A plot of the solution to the boundary value problem ey'' + y' $_{=}O$, y(0) = O, y(l) = 1. This is a singular perturbation problem because the curve in the boundary-layer region becomes steeper as $_{\pm}$ approaches zero and becomes discontinuous when $_{\pm}$ reaches zero. The boundary layer region extends from x = 0 to $x \simeq \epsilon$.

ing our new perturbative techniques. Nearly all boundarylayer problems are differential equation problems in which the highest derivative term is multiplied by a small parameter. A simple mathematical example will explain the appearance of a boundary layer.

Consider the boundary-value problem

$$\varepsilon \frac{d^2 y}{dx^2} + \frac{dy}{dx} = 0$$
, $y(0) = 0$, $y(1) = 1$. (5)

The exact solution to this problem is

$$y(x) = \frac{1 - e^{-x/\epsilon}}{1 - e^{-1/\epsilon}}$$

its graph for various values of ε is shown in Fig. 2. As ε decreases the curve becomes steeper in the region from x = O to $x \cong \varepsilon$. This region, in which y(x) exhibits transient behavior or rapid variation, is called a boundary layer. In fact, y(x) becomes discontinuous as ε decreases to zero. Equation (5) is a singular perturbation problem because the order of the differential equation changes abruptly from 2 to 1 as $\varepsilon \to 0$. Since a first-order differential equation cannot satisfy two independent boundary conditions. the solution ceases to exist when $\varepsilon = O$ and a discontinuity appears in y(x).



Conventional Solutions

A review of the well-known conventional methods for obtaining the first approximation (the first term in the perturbation series) to the solution of a very general boundarylayer problem provides a contrast to our radically new approach.

We consider a boundary-value problem of the form

$$z \frac{d^2 y(x)}{dx^2} + a(x) \frac{dy(x)}{dx} + b(x)y(x) = 0, \ y(0) = A, \ y(1) = B,$$
(6)

where ε is a small positive parameter. This equation is a generalization of Eq. (5). A and B are arbitrary numbers, and a(x) and b(x) are completely arbitrary continuous functions of x. From boundary-layer theory, we know that if a(x) is nonzero, the term a(x) [dy(x)/dx] acts as a "friction" force, which results in a boundary layer. If a(x) > 0 for $0 \le x \le 1$ (positive damping), the boundary-layer occurs immediately at x = 0. If a(x) < 0, the boundary layer occurs at x = 1. In general, the thickness of a boundary layer is determined by a scaling transformation on the differential equation. For Eq. (6) with a(x) positive, the boundary layer has thickness ε and lies in the region x = 0 to $x \simeq \varepsilon$. (See Fig. 3.) Although Eq. (5) [a special case of Eq. (6)] is simply solvable, in general Eq. (6) has no closed-form analytic solution. As with the quintic polynomial in Eq. (1), we must use perturbation methods to obtain an approximate solution.

To solve the boundary-value problem in Eq. (6) approximately for small ε , we make several inspired observations, which allow us to approximate the solutions inside and outside the boundary-layer region and to match these solutions. First, we consider the boundary-layer region where the solution y(x) varies rapidly and is very steep. To be precise, scaling arguments. referred to above tell us that a(x) [dy(x)/dx] is much larger than b(x)y(x) in the boundary-layer region (order 1/& compared with order 1). (See Fig. 2.) Moreover, since the boundary layer from x = 0 to $x \cong \varepsilon$ is very narrow, we can approximate the function a(x) by a(0). Hence, inside the boundary-layer region, we may replace Eq. (6) by the much simpler equation

$$\frac{\mathrm{d}^2 \mathbf{y}(\mathbf{x})}{\mathrm{d}\mathbf{x}^2} + \mathbf{a}(0) \frac{\mathrm{d}\mathbf{y}(\mathbf{x})}{\mathrm{d}\mathbf{x}} = 0 \ (0 \le \mathbf{x} \le \varepsilon) \ . \tag{7}$$

Equation (7) is easy to solve because it is a constant-coefficient equation. The solution that passes through A at x = O is

$$\psi(\mathbf{x}) = (\mathbf{A} - \mathbf{C}) \exp[-\mathbf{a}(\mathbf{0})\mathbf{x}/\mathbf{\epsilon}] + \mathbf{C} \ (\mathbf{0} \le \mathbf{x} \le \mathbf{\epsilon}) \ ,$$
 (8)

where C is an arbitrary constant.

Second, we consider the region outside the boundary layer, where y(x) varies very slowly. Thus, $\varepsilon d^2y(x)/dx^2$ is small compared with a(x) dy(x)/dx + b(x)y(x), and we may replace Eq. (6) by the first-order equation

$$a(x)\frac{dy(x)}{dx} + b(x)y(x) = 0 \quad (\varepsilon \le x \le 1) .$$
(9)

The solution that passes through B at x = 1 is

$$y(\mathbf{x}) = \mathbf{B} \exp\left[\int_{\mathbf{x}} d\mathbf{t} \ \mathbf{b}(\mathbf{t})/\mathbf{a}(\mathbf{t})\right] \ (\varepsilon < \mathbf{x} < 1) \ . \tag{10}$$

To determine C in Eq. (8) we use the sophisticated perturbative method called asymptotic matching. Roughly speaking, we demand that Eqs. (8) and (10) agree in the region just to the right of the boundary layer, say at x = -&. This gives

$$C \cong B \exp\left[\int_{0}^{1} dt b(t)/a(t)\right]$$
.

A simple and elegant expression combines the results in Eqs. (8) and (10) to give a good uniform approximation to y(x) over the entire region $0 \le x \le 1$.

$$y(x) = \left(A - B \exp\left[\int_{0}^{1} dt \ b(t)/a(t)\right]\right) \exp\left[-a(0)x/\epsilon\right]$$

+ B $\exp\left[\int_{x} dt \ b(t)/a(t)\right]$ (11)

The expression in Eq. (11) differs from the exact solution to Eq. (6) by terms of order ε . (See Fig. 3.)

This conventional approach to the solution of boundary-



Fig. 3. A schematic comparison between the exact solution of the general linear boundary-layer problem in Eq. (6) and the leading-order uniform approximation to the exact solution in

layer problems is widely known and well used, However, even the approximate equations that must be solved inside or outside the boundary layer cannot be solved analytically in some cases. Differential equations that are nonlinear or higher than second order present such difficulties; ordinarily they are solved numerically on a computer. With our new methods, these problems can be solved without recourse to large computer codes.

And Now For Something Completely Different

Our approach to boundary-layer problems is quite different; we will actually solve a singular boundary-layer problem as a regular perturbation problem. The approach has two parts. First, we replace the differential equation by a difference equation on a lattice. The replacement allows us to express the

Eq. (11). The approximate solution differs from the exact solution by terms of order ε . The boundary-layer region extending from x = 0 to $x \cong \varepsilon$ is shown.

solution as a regular perturbation series in powers of ε as long as the lattice spacing a is held fixed and finite. Second, we take the lattice spacing a to zero to recover the answer to the original problem in the continuum. However, this limit is very peculiar because, as the lattice spacing goes to zero, the perturbation parameter ε goes to infinity. The perturbation series originally obtained in the limit of small ε is now infinite term by term. We use clever summation techniques to determine a finite answer—an answer that approximates the behavior in the boundary layer to surprisingly good accuracy.

We present the new perturbative methods in an application to the nonlinear two-dimensional wave equation for the function u(x,t).

$$\epsilon^2 \, \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial t^2} + u - u^3 = 0 \; .$$

The equation has a static solution, called a kink, whose analytical form is

$$u(\mathbf{x}) = \tanh \frac{\mathbf{x}}{\varepsilon \sqrt{2}} \tag{12}$$

The kink solution solves the boundary-value problem

$$\varepsilon^2 \frac{d^2 u}{dx^2} + u - u^3 = 0, u(0) = 0, u(+\infty) = 1$$
. (13)

We know that Eq. (13) is a singular perturbation problem because the highest derivative in the equation is multiplied by ε [as are the highest derivatives in Eqs. (5) and (6)]. Also, the kink solution Eq. (12) exhibits typical boundary-layer structure; u(x) varies slowly except in the boundary-layer region $-\varepsilon \le x \le \varepsilon$, where it rapidly goes from -1 to l. (See Fig. 4.)

To find u(x) we begin by changing the differential equation to a difference equation. That is, we consider space to be made up of a lattice of distinct points with the spacing a between them held fixed. The points x are denoted by na (n = O, 1,2, ...) and u(x) becomes $u(na) = U_n$. The derivatives of u on the lattice become finite differences; in particular,

$$\frac{d^2 u(x)}{dx^2} = \frac{1}{a^2} \left(u_{n+1} - 2u_n + u_{n-1} \right).$$

The difference equation for Eq. (13) is thus

$$\frac{\varepsilon^{2}}{a^{2}}(u_{n+1}-2u_{n}+u_{n-1})+u_{n}-u_{n}^{3}=0, u_{0}=0, u_{\infty}=1.$$
(14)

In the first part of our approach, we hold the lattice spacing a fixed while we solve Eq. (14) perturbatively for small ε . With a held fixed and ε small, the natural expansion parameter for the problem is

 $\mathfrak{z} = \epsilon^2/a^2$.

We therefore expand u_n for each value of n as a power series in \mathfrak{z} ,

$$a_n = a_n + b_n \delta + c_n \delta^2 + d_n \delta^3 + \dots , \qquad (15)$$



Fig. 4. The so-called kink solution to the equation $\varepsilon^2 u_{xx} + u - u^3 = 0$, u(0) = 0, $u(+\infty) = 1$. Observe that u(x) rapidly goes from -1 to 1 in the boundary-layer region when ε is small.

just as we did in Eq. (3) for the regular perturbation problem in Eq. (2).

We impose the initial conditions by taking

$$a_n = \begin{array}{c} O \text{ if } n = O ,\\ \text{ if } n \ge 1 . \end{array}$$

Note that these conditions solve the unperturbed problem $(\delta = 0)$ and thus follow the usual approach in regular perturbation problems. Substituting Eq. (15) into Eq. (14) and comparing powers of δ , just as we did in solving Eq. (2), routinely gives the perturbation coefficients. The u_a at the first few points on the lattice near x = O are

$$\begin{aligned} \mathbf{u}_{0} &= 0 \\ \mathbf{u}_{1} &= 1 - \frac{1}{2} \,\delta + \frac{1}{8} \,\delta^{2} &+ \frac{11}{28} \,\delta^{4} \\ \mathbf{u}_{2} &= 1 &- \frac{1}{4} \,\delta^{2} + \frac{5}{16} \,\delta^{3} - \frac{15}{32} \,\delta^{4} \\ \mathbf{u}_{3} &= 1 &- \frac{1}{86} \,\delta^{3} + \frac{9}{32} \,\delta^{4} \\ \mathbf{u}_{4} &= 1 &- \frac{1}{16} \,\delta^{4} \,, \end{aligned}$$
(16)

where we have calculated u_n to the fourth order in δ and have lined up the contributions according to the order of the perturbation expansion in which the terms appear. (If k is the order of the expansion, the matrix $\frac{k_1}{k_1}$ is triangular for k > 1)



Fig. 5. The development of the boundary-layer structure as the order of the perturbation expansion increases. Results for u_n are plotted in zeroth-, first-, and second- order perturbation theory before taking the limit $\delta \rightarrow 0$. (For this plot we chose $\delta = 1$ and $a = \varepsilon = 1/4$.) Compare these results to the exact solution plotted in Fig. 4.

The boundary structure develops as we go to higher orders of the perturbation expansion (higher powers of δ). We determine one point in the boundary layer in the first order, two points in the second order, three points in the third order, and so on. (See Fig. 5.)

It is a peculiarity of our method that the thickness of the boundary layer is na in nth-order perturbation theory, and the boundary layer vanishes in the limit of zero-lattice spacing

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 $(a \rightarrow 0)$. Since all the points u_n shrink to the origin as $a \rightarrow 0$, we cannot determine the value of u(x) in the boundary layer by taking the continuum limit of Eq. (15) directly. However, the derivatives of u(x) at the origin are defined in this limit and can be determined from the usual definitions,

$$u'(0) = \lim_{a \to 0} \frac{u_1 - u_0}{a},$$
$$u''(0) = \lim_{a \to 0} \frac{u_1 + u_{-1} - 2u_0}{a^2}$$

and so on. In many cases, the derivatives themselves are of physical interest, and further, we can reconstruct the function in the boundary layer from its Taylor series.

$$u(x) = \sum_{n=0}^{N} u^{(n)}(0) \frac{x^n}{n!}$$

where

$$u^{(n)}(x)=\frac{d^nu(x)}{dx^n}.$$

How well can we determine the first derivative at the origin u'(0) from Eq. (14)? From the exact solution given by Eq. (12) *we* know that

$$u'(o) = \frac{1}{\varepsilon\sqrt{2}} = 0.7071 \text{ ve}.$$
 (17)

Using the expansions in Eq. (16), we have the following result for the first derivative at the origin.

$$\mathfrak{u}'(0) = \lim_{a \to 0} \frac{1}{a} \left(1 - \frac{1}{a} + \frac{1}{a} + \frac{1}{a} + \frac{1}{a} \delta^4 + \dots \right) \,.$$

In the limit as $a\to 0,\,\delta$ is no longer small; in fact, $\delta=\epsilon^2/a^2$ goes to infinity and

$$\mathbf{u}'(0) = -\lim_{n \to \infty} \sqrt{\delta} \left(1 - \frac{1}{2} + \frac{1}{2} + \frac{1}{22} \delta^4 + \ldots\right). \tag{18}$$

The factor $1/\varepsilon$ in Eq. (18) agrees with the $1/\varepsilon$ in the exact result in Eq. (17). But does the limit of the series in Eq. (18) give $1/\sqrt{2}$? This limit should be understood as follows: our perturbation series has been derived by assuming that a is fixed and that ε and therefore δ are small. Now we must return to the continuum problem in Eq. (13) by taking a + O and keeping ε fixed; therefore we must take the limit $\delta \rightarrow \infty$. Apparently we have a disaster—all terms in Eq. (18) diverge, and what is more, each new term approaches infinity faster than the preceding term because it has two additional powers of a in its denominator.

Everything has been routine until now; why do such unpleasant difficulties arise? The answer is that we have been treating what is fundamentally a singular perturbation problem as a regular perturbation problem by seeking perturbation series in the form of Taylor series [Eq. (5)], and the mathematics is trying to make us pay for our naivety. We will return to Eq. (18) after we have resolved this difficulty.

How To Sum The Series $\infty + \infty + \infty + \infty + \dots$ And Get a Finite Answer

An elementary example will explain how the series in Eq. (18) can have a finite sum in the limit $a \rightarrow 0$. Suppose we are asked to expand \sqrt{x} in a Taylor series about x = 0. The request seems unreasonable because this function does not have such a series (all derivatives of \sqrt{x} are singular at x = 0). Nevertheless, we have an idea. We introduce a lattice spacing a and consider the function $(x + a)^{1/2}$, which does have a Taylor series about x = 0.

$$[\mathbf{x} + \mathbf{a})^{1/2} = \mathbf{a}^{1/2} + \frac{\mathbf{x}}{2\mathbf{a}^{1/2}} - \frac{\mathbf{x}^2}{8\mathbf{a}^{3/2}} + \dots \quad (19)$$

In the limit $a \rightarrow 0$ every term after the first becomes infinite, just as in Eq. (18), but the *sum* of the series is not necessarily infinite. Indeed, if we sum the series first, we obtain $(x + a)^{1/2}$; hen we can take the limit $a \rightarrow 0$ and obtain the finite answer \sqrt{x} .

Thus we would like to sum the series in Eq. (18) before we **ake the limit a** \rightarrow 0 or $\delta \rightarrow \infty$. Although we know all the terms in the series in Eq. (19), we know only a finite number, say N + 1, of terms in Eq. (18). If we know only N + 1 terms, how can we trick the series in Eq. (18) into revealing its approximate finite sum?

We have developed a general procedure for summing a series with N + 1 terms. Suppose we calculate a quantity $Q(\varepsilon)$ as a series in powers of ε .

$$Q(\varepsilon) = \varepsilon^{\alpha} \sum_{n=0}^{\infty} a_n \varepsilon^n , \qquad (20)$$

where **a** is an arbitrary nonnegative exponent. Here we have generalized the notion of a Taylor series slightly to include the possibility of an overall multiplicative fractional power of ε . This series is just like the series in Eq. (18) if we set $\varepsilon = \delta$ and a = 1/2. Now we can calculate Q(m) knowing only N + 1 terms in the series, if we know that Q(∞) is finite.

We proceed to manipulate the series in Eq. (20) until we create a structure that has a finite limit as $\varepsilon \rightarrow \infty$. First, we raise both sides of Eq. (20) to the power l/a.

$$Q(\varepsilon)^{1/\alpha} = \varepsilon \sum_{n=0}^{\infty} (a_n \varepsilon^n)^{1/\alpha}.$$

Using the usual rules for exponentiating a Taylor series, we can rewrite $Q^{1/\alpha}$ in the following form.

$$Q(\varepsilon)^{1/\alpha} = \varepsilon \sum b_n \varepsilon^n$$
$$= \frac{\varepsilon}{\sum c_n \varepsilon^n}.$$

Finally, we raise this equation to the integer power N,

$$Q(\varepsilon)^{N/\alpha} = \frac{\varepsilon^{N}}{\sum\limits_{n=0}^{\infty} C_{n}^{(N)} \varepsilon^{n}}.$$
(21)

For all these Taylor series manipulations, we assume & is small.

Since we know only N + 1 terms in the series in Eq. (20), we must work consistently and truncate the series in Eq. (21) at n = N. Now we have a structure that is well-defined in the limit $: \rightarrow \infty$; in fact, as $\epsilon \rightarrow \infty$, the only term that survives is $/C_n^{(N)}$.

$$\lim_{\epsilon \to \infty} Q(\epsilon)^{N/\alpha} \sim \lim_{\epsilon \to \infty} \frac{\epsilon^{N}}{\sum\limits_{n=0}^{N} C_{n}^{(N)} \epsilon^{n}} = \frac{1}{C_{N}^{(N)}}$$

Thus we have obtained an approximate value for $Q(\infty)$, which we call Q_N .

$$\mathsf{D}_{\mathsf{N}} = [\mathsf{C}_{\mathsf{N}}^{(\mathsf{N})}]^{-\alpha/\mathsf{N}} \ . \tag{22}$$

We refer to Q_N as the Nth approximant to Q(m); in many problems Q_N tends to $Q(\infty)$ as $N \to \infty$. More importantly, in most problems Q_N rapidly gets very close to $Q(\infty)$ when N is still quite small. Through a sequence of simple series manipulations we have converted the series in Eq. (20), which is meaningless as $z \to \infty$, into a series of well-defined extrapolants Q_N .

An Example

The convergent properties of the extrapolants Q_{N} are so surprising that we must demonstrate them with a specific example. The transcendental equation

in
$$x + \frac{1}{1-x} = 0$$
 (23)

has one root between O and 1:

 $x = 0.2592463566483 \dots$

Let us see if we can obtain this root perturbatively. We begin by introducing a perturbation parameter E in a most unusual way.

in
$$x + \frac{1}{1+\frac{1}{2}} (\frac{\varepsilon}{1-x} + 1) = 0.$$
 (24)

We have chosen to introduce ε this way for two reasons. First, the original equation in (23) is recovered in the limit $\varepsilon \to \infty$. Second, the unperturbed problem [Eq. (24) with E = O] is easy to solve: $\ln x + 1 = 0 \to x = 1/e$. With this solution for the unperturbed problem we proceed to find the rest of the perturbation series for E # O by the iterative methods discussed earlier for regular perturbation problems. The series for the root $_{x(E)}$ to Eq. (24) is

$$\mathfrak{c}(\varepsilon) = \frac{1}{\varepsilon} (1 - 0.58198\varepsilon + 1.28714\varepsilon^2 - 3.16768\varepsilon^3 \dots) \,. \tag{25}$$

We would like to sum this series as $\varepsilon \to \infty$ using the general formula in Eq. (22), which requires that $\alpha \neq 0$. To convert the series to a form in which a = 1, we multiply Eq. (25) by e, take the natural logarithm, and multiply by -1.

$$Q(\varepsilon) = -\ln[e \ x(\varepsilon)]$$

= $\varepsilon (0.58198 + 1.11779\varepsilon + 2.48430\varepsilon^{2} - 6.26489\varepsilon^{3} + ...)$ (26)

The extrapolants for Eq. (26) defined by Eq. (22) yield a very rapidly convergent sequence for the roots of the transcendental equation in Eq. (23).

which is now correct to one part in 10^8 .

Note that the extrapolants Q_N , which are all positive, are derived from a perturbation expansion that has both positive and negative terms. The remarkable fact that the first N coefficients in the series raised to the Nth power are all positive ensures that the extrapolants Q_N are always real.

a spin-off from PARTICLE PHYSICS RESEARCH

O ur new techniques for singular perturbation problems were developed to solve mathematical problems that arise in a field-theoretic treatment of strongly interacting particles. Strong forces mean that the parameter describing the interactions between particles is very large compared to other parameters in the problem. This problem is very different from the weak-coupling problems usually studied (such as those arising in quantized electromagnetic interactions), in which the interaction force is small (weak) and thus can be treated as a perturbation on a system of freely moving, noninteracting particles. The answers to weak-coupling problems are expressed as power series in the strength of the small interaction force.

In the strong-coupling case, we cannot treat the interaction term as a perturbation since it dominates the dynamics. Instead, we treat the kinetic energy term that determines the motion of free particles as the perturbation. The unperturbed system now consists of particles that interact through strong forces but are motionless or frozen in space time.

The strong-coupling or kinetic energy expansion is singular because the kinetic energy can become arbitrarily large. As a result, the terms in the perturbation expansion in inverse powers of the coupling strength are not well defined. To proceed we use an artifice: we model space-time as a lattice of discrete points rather than as a continuum. This trick, commonly used in particle physics, prevents the momentum or kinetic energy from becoming

arbitrarily large. Particle motion is no longer continuous but rather consists of hopping from site to site. Although the dynamics on the lattice is unfamiliar, the strong-coupling expansion of physical quantities becomes well defined and very easy to compute, so easy that the computations are purely algebraic and we can program computers to do the manipulations to a very high order in the perturbation expansion. However, the introduction of a space-time lattice has a major drawback; it introduces into the problem an artificial length, namely, the lattice spacing a between lattice sites. To obtain physically meaningful results, we must return to the continuum by taking the lattice spacing *a* to zero. Performing this singular and difficult limit was a central problem we solved in our research.

We now realize that the introduction of a lattice and the subsequent continuum limit $a \rightarrow 0$ is a powerful mathematical tool that can be applied to many singular perturbation problems outside the realm of quantum field theory. In general, it has the advantage of converting *singular* perturbation problems that require a great deal of mathematical subtlety and ingenuity into *regular* perturbation problems whose iterative solutions are straightforward and routine. We have used these methods to solve a variety of singular perturbation problems, and we have even used them to elucidate the statistical mechanics of randomly driven nonlinear oscillators

Why Equation (22) Works

We can develop some intuition for why Eq. (22) defines a convergent series of approximants by doing a saddle-point evaluation of a complex integral. For those not interested in this argument, skipping to the next subheading will not break the continuity of our presentation.

If f(z) is an analytic function in a region of the complex-z plane containing the origin, the nth term in the Taylor series for

$$f(z) = \sum_{n=0}^{\infty} A_n z^n$$

is given by a contour integral,

$$A_n = \frac{1}{2\pi i} \int_C \frac{f(z)}{z^{n+1}} dz$$
,

where the contour C encircles the origin. Hence, after making some reasonable analyticity assumptions, we may use this formula to solve Eq. (21) exactly for $C_N^{(N)}$.

$$C_{N}^{(N)} = \frac{1}{2\pi i} \int_{C} \frac{d\epsilon}{\epsilon} Q(\epsilon)^{-N/\alpha} . \qquad (27)$$

We would like to examine the behavior of $C_N^{(N)}$ for large N to see if the sequence of approximants converges. To do so, we rewrite the integrand as

 $\exp[-N \ln Q(\epsilon)/\alpha]$.

For large N, we apply the saddle-point method. A saddle point $\&_{\rm o}{\rm is}$ defined by the condition

$$Q'(\varepsilon_0) = 0 {.} {(28)}$$

We shift the contour C in Eq. (27) until it passes through the saddle point ε_0 (assuming for now that there is only one) and for the sake of simplicity we ignore any contributions that might come from passing the contour through a singularity in

the complex-s plane. The saddle-point method tells us that the most important contribution to the integral in Eq. (27) is found by evaluating the integrand at the saddle point ε_0 . (We will ignore any terms that depend on N algebraically because, as we will see, we are going to take the Nth root of the result and let N tend to infinity; in this limit all algebraic terms approach 1.) Evaluating the integral at the saddle point gives

$$C_N^{(N)} \cong \frac{1}{2\pi i} \frac{1}{\epsilon_0} \, Q(\epsilon_0)^{-N/\alpha} \; . \label{eq:CN}$$

Using the definition of the extrapolants Q_{N} in Eq. (21), we have

$$Q_{N} = \begin{bmatrix} C_{N}^{(N)} \end{bmatrix}^{-\alpha/N} = \left(\frac{1}{2\pi i} \frac{1}{\varepsilon_{0}}\right)^{-\alpha/N} Q(\varepsilon_{0})$$

Thus we have $Q_N \cong Q(\epsilon_0)$, where the error approaches zero as $N \to \infty$. Hence,

$$\lim_{N\to\infty} Q_N = Q(\varepsilon_0) \; .$$

This result may seem very disappointing at first because we were hoping that

 $\lim_{N\to\infty} Q_N = Q(\infty) \; .$

However, we assumed at the start that Q(m) was finite. This is roughly the same as assuming that $Q(\varepsilon)$ is level at $\varepsilon = \infty$, which means that it smoothly approaches the constant $Q(\infty)$] and thus satisfies the saddle-point condition Eq. (28) at $\varepsilon_0 = \infty$. In effect, we have assumed at the start that $\varepsilon_0 = \infty$ is a saddle point. Now we understand why the formula Eq. (22) can produce a series of approximants that actually approach $Q(\alpha)$).

This argument also explains why Eq. (22) sometimes fails; it can fail if there is another saddle point in the complex-c plane that gives a larger contribution than the one at ∞ .

Here is the surprising part: although there are many problems for which the sequence of approximants Q_N doesn't converge to Q(m), in all 25 or so problems that we have investigated, both in quantum-field theory and in boundary-layer theory, the Q_N sequence still gives a remarkably accurate approximation to the exact answer. Sometimes the approximants Q_N come very close to the exact answer and then veer away, just like the partial sums of an asymptotic series. We do not really understand yet why our method works so well.

Back To The Kink . . .

Now that we have described a general method for extrapolating series like the one in Eq. (18) to the continuum, we will return to the kink problem and see how well our method works. The exact answer for the series in Eq. (18) is $1/(\epsilon\sqrt{2})$, given by Eq. (17). Thus, we would like the series in powers of δ to approach $1/\sqrt{2}$ as $\delta \rightarrow \infty$. We use the general formula in Eq. (22) with a = 1/2 to obtain the following sequence of approximants.

The extrapolants are already very close to the exact answer 0.70711. The higher extrapolants continue to decrease monotonically until a surprising thing happens; they undershoot the exact answer and continue decreasing until they reach a minimum in 24th order.

 $Q_{24} = 0.70198$,

The relative error between this value and the exact answer is less than 1%. The extrapolants gradually rise monotonically until they recross the exact answer in 41st order; we believe that the extrapolants will continue to rise from here on. Unlike the example in Eq. (23), the sequence of approximants is not convergent, probably because of the effect of a saddle point. Nevertheless, the sequence is asymptotic in nature; like Stirling's series for the gamma function and other asymptotic series, early terms in the series comprise a good approximation to the answer until some optimal order is reached. Afterwards, the direct approximants from these series diverge.*

In the same way that we determined u'(0), we can determine all the derivatives $U^{(*)}(0)$ for Eq. (18) by extrapolating series expansions of the form

Then, we can use the Taylor series for u(x) for $x < x_0$ where $u(x_0) = 1$, and we can set u(x) = 1 for $x \ge x_0$ to get a reasonable global reconstruction of u(x). However, we need to know at least 10 terms in the Taylor series to perform this reconstruction.

The method we have described to determine u(x) relies on obtaining local information for the differential or classical field equation at the origin. In his paper, "Singular Perturbation-Strong Coupling Field Theory," Carlos R. Handy, a Postdoctoral Fellow at Los Alamos, developed an alternative approach, which allows for global reconstruction of the field solution. The method combines two mathematical tools. The first is the lattice expansion for the given field equation; an example is Eq. (15), from which the power moments are determined as an expansion in inverse powers of the lattice spacing. Handy uses Pade approximant techniques to obtain approximate continuum limit power moments. The second relates to the traditional, mathematical "moments problem." After obtaining a sufficient number of the approximate continuum moments, he reconstructs the corresponding approximate global field solution. This procedure gave excellent results for both the +4-classical field theory kink and the Sine-Gordon equation kink solutions. It is equivalent to a momentum space formulation of the problem in which the long-range, large-scale behavior of the fields is determined by the small-momentum infrared domain.

^{*}The perturbation series derived from conventional boundary-layer methods are also asymptotic divergent series.

Other Boundary-Layer Problems

Boundary layers or transient phenomena arise in many diverse physical settings. Here we apply the new solution techniques to three problems.

1. Blasius Equation

The Blasius equation describes the boundary-layer structure of fluid flow across a flat plate.

$$2\varepsilon y'''(x) + y(x)y''(x) = 0, y(0) = y'(0) = 0, y'(+\infty) = 1$$

A quantity of physical interest is y"(0), which determines the stress on the plate apart from dimensional parameters.

To solve for y''(0) perturbatively, we rewrite the Blasius equation on a lattice.

$$2\delta(f_{n+1} - 3f_n + 3f_{n-1} - f_{n-2}) + f_n(f_{n+1} - 2f_n + f_{n-1}) = 0 \ ,$$

where $f_n = y(na)/a$, $\delta = \epsilon/a^2$, and a is the lattice spacing. As usual, we solve for f_n as a series in powers of δ and obtain from the solution a sequence of extrapolants for y"(0). The exact value for y"(0) obtained numerically is (0.33206...) $\sqrt{\epsilon}$. The first few extrapolants obtained by our new techniques are

 $\begin{array}{l} Q_1 = 0.5/\sqrt{\epsilon} \;, \\ Q_2 = 0.4204/\sqrt{\epsilon} \;, \\ Q_3 = 0.3948/\sqrt{\epsilon} \;, \\ Q_4 = 0.3819/\sqrt{\epsilon} \;, \text{ and} \\ Q_5 = 0.3742/\sqrt{\epsilon} \;. \end{array}$

As N increases, Q_N becomes very flat.

 $\begin{array}{l} Q_{25}=03502/\sqrt{\epsilon}\;,\\ Q_{26}=0.3500/\sqrt{\epsilon}\;,\\ Q_{37}=0.3485/\sqrt{\epsilon}\;,\text{ and}\\ Q_{38}=0.3484/\sqrt{\epsilon}\;. \end{array}$

The relative error between the exact answer and Q_{ss} is about 5%. At present, we do not know whether the sequence Q_N approaches the exact answer as $N \to \infty$. In fact, there are many ways to extrapolate Q_N to its limiting value Q_{∞} , but we

2. Damped Linear Oscillator

An initially quiescent spring-mass system subject to an impulse 1_0 at t = O satisfies the equation

$$m \frac{d^2 y}{dt^2} + \beta \frac{d y}{dt} + k y = I_0 \delta(t) , \ y(0_-) = y'(0_-) = 0 ,$$

where 13 is the damping coefficient, m is the mass, and k is the spring constant. For small m, the solution y(t) exhibits a boundary layer of thickness m/~ situated at t = O. The exact solution satisfies $y'(O^{*}) = 1_{0}/m$.

The lattice version of the differential equation is

$$\epsilon(y_{n+1} - 2y_n + y_{n-1}) + y_{n+1} - y_n + kay_n/\beta = I_0 \delta_{n,0}/\beta$$

where $y(an) = y_n$ and $\varepsilon = n/(\beta a)$. On the lattice the perturbation series for the damping term at t = 0, y'(0), is very simple.

$$y'(0) = \lim_{\epsilon \to \infty} \epsilon \frac{I_0}{m} (1 - \epsilon + \epsilon^2 - \epsilon^3 ...) .$$

Using Eq. (22), the formula for the Nth approximant Q_N , we obtain for all N

$$Q_{N} = \frac{I_{0}}{m}.$$

Thus, our perturbative approach gives the exact answer to all orders.

3. Green's Function for the Diffusion Equation

Our lattice techniques work for partial as well as for ordinary differential equations. To illustrate, we consider a heat diffusion equation with a point source in the space and time variables.

 $u_t = \upsilon u_{xx} + \delta(t)\delta(x) , u(x,t) = 0 (t < 0) ,$

where v is the thermal diffusivity. The solution to this equation u(x,t) describes the temperature distribution in a onedimensional system like a wire or rod.

will not discuss them here.

The exact solution is the Green's function,

$$J(\mathbf{x},t) = \frac{\theta(t)}{(4\pi v t)^{1/2}} \quad \exp(-x^2/4\pi v t) , \qquad (29)$$

where

$$\vartheta(t) = \frac{1 \text{ if } t \ge 0}{0 \text{ if } t < 0}$$

Note that for small v and fixed t, the temperature distribution u(x,t) has a boundary layer of thickness $(vt)^{1/2}$ at x = O. We wish to calculate the temperature at x = O and time t. The exact result from Eq. (29) is

$$u(0,t) = \frac{\theta(t)}{(4\pi \upsilon t)^{1/2}} = (0.282095) \frac{\theta(t)}{(\upsilon t)^{1/2}}.$$

To apply our solution methods, we introduce a discrete lattice in the spatial variable to obtain the differentialdifference equation

$$\frac{d}{dt}u_n = \epsilon(u_{n+1} - 2u_n + u_{n-1}) + \frac{\delta(t)\delta_{n,0}/a}{a},$$

where $\varepsilon = \upsilon/a^2$. The perturbation series solution for u_0 , the temperature at x = O, is

$$u_{0}(t) = \lim_{a \to 0} \frac{1}{a} \theta(t) \sum_{k=0}^{\infty} \frac{(-\epsilon t)^{k} (2k)!}{(k!)^{3}}$$
$$= \frac{\theta(t)}{(\nu t)^{1/2}} \lim_{\epsilon t \to \infty} (\epsilon t)^{1/2} \sum_{k=0}^{\infty} \frac{(-\epsilon t)^{k} (2k)!}{(k!)^{3}}.$$

This series can be summed exactly to give

$$u_0(t) = \theta(t) (\varepsilon/\upsilon)^{1/2} \exp(-2t\varepsilon) I_0(2t\varepsilon) ,$$

where 1_0 is an associated Bessel function, Using the asymptotic relation $I_0(x) \sim e^{x}/(2\pi x)^{1/2} (x \to +\infty)$, we can take the limit $\varepsilon \to \infty$ to obtain the exact answer in Eq. (29).

However, we are more interested in finding out what happens when we extrapolate the perturbation series term-by-term to the limit using Eq. (22). We obtain a sequence of extrapolants, which appear to converge rather slowly after they have been divided by $\theta(t)/(tt)^{1/2}$.

$$Q_1 = 0.5,$$

 $Q_2 = 0.435,$
 $Q_3 = 0.408,$
 $Q_4 = 0.393,$ and
 $Q_5 = 0.384.$

The sequence continues to approach the exact answer but becomes very flat as N increases.

$$Q_{10} = 0.362,$$

$$Q_{15} = 0.354,$$

$$Q_{20} = 0.349,$$

$$Q_{25} = 0.346,$$

$$Q_{30} = 0.344,$$

$$Q_{35} = 0.343,$$
 and
$$Q_{40} = 0.342.$$

The last approximant differs from the exact answer by about 18%. This example gives the poorest results we have found so far; in most problems we have studied, we can predict the answer to within a few percent.

Conclusions

Our new way of doing perturbation theory, in which the perturbation parameter ε initially is assumed to be small and eventually is extrapolated to infinity, appears to be a powerful tool in boundary-layer theory and in many other areas. Although the method involves taking unusual limits, the computations are purely algebraic and therefore relatively simple. There is much work to be done in determining the method's full range of applicability. We have returned to its application in field theory and hope that investigators in other areas will find ways to exploit the methods in new physical contexts

THE AUTHOR



Carl Bender, Visiting Staff Member in the Laboratory's Theoretical Division, is a Professor of Physics at Washington University. He received his A.B. from Cornell University in 1964, his Ph.D. in Theoretical Physics from Harvard University in 1969, and held a one-year postdoctoral appointment at the Institute for Advanced Study in Princeton. Until [977 he was an Associate Professor of Applied Mathematics at Massachusetts Institute of Technology where he received the Graduate Teaching Award in 1976. He was awarded a Sloan Foundation Fellowhip in Theoretical Physics and Applied Mathematics. Preciously. he was a visiting Research Scientist at Imperial College. London, and at California Institute of Technology. He has published widely in the fields of Applied Mathematics and Theoretical Physics. Currently he is on the Editorial Board of Advances in Applied Mathematics. He is coauthor of Advanced Mathematical Methods for Scientist and Engineers. which is used as a standard text for graduate scientists.

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