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ASYMPTOTIC APPROXIMATIONS TO THE SOLUTION OF THE HEAT EQUATION

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ABSTRACT. In one-dimensional problems of diffusion or heat conduction where discontinuities or steep gradients occur in the initial or boundary conditions a singular perturbation analysis can give accurate estimates of the solution when numerical methods prove inefficient or inadequate. In fact, the discontinuities can be exploited in the singular perturbation analysis to obtain an asymptotic series representation of the solution.

Several different problems of increasing complexity can be explicitly solved when the boundary and initial data are given in piecewise polynomial form: (a) infinite region or pure initial value problem, (b) semi-infinite region, and (c) finite region.

The approximate methods also apply to the case when no discontinuities occur in the prescribed data or its derivatives.

1. **Introduction.** It is frequently stated in regard to heat conduction and diffusion problems that "discontinuities are immediately damped out". In some problems arising in engineering, however, this view is too over-simplified to be realistic because the damping out process itself is the heart of the problem. Typically, such problems exhibit a behavior usually referred to as "very steep gradients" which present severe difficulties to attempted solution by numerical techniques; viz., very small mesh sizes and excessive roundoff errors. We shall examine in this paper how such problems are most suitably handled by a singular perturbation analysis. The analysis will show how very accurate estimates of the solution can be obtained with just a few easily calculated terms.

We first wish to give an example of the type of problem we have in mind, namely, heat conduction in rifle barrels. We assume circular symmetry and independence of the axial coordinate. The phenomenon is then described by the heat conduction equation in radial coordinates:

$$u_t = a[u_{rr} + (1/r)u_r].$$

The radial coordinate varies from r_0 = interior radius of the barrel to r_1 = exterior radius. The initial and boundary (radiation) conditions are

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$$u(r, 0) = \text{ambient temperature},$$
$$u(r_0, t) + h_0 u_r(r_0, t) = \text{propellant gas temperatures at time } t,$$
$$u(r_1, t) + h_1 u_r(r_1, t) = \text{ambient temperature},$$

where h_0 and h_1 are heat transfer coefficients. The coefficient of thermal diffusivity, a, for mild steel is 0.12 cm^2/sec. A typical length scale in this problem is $r_1 - r_0$ which is on the order of 1 cm. A typical time scale is the duration of the phenomenon which is on the order of 1 millisecond. In non-dimensional form then the coefficient a is on the order of 10^{-4}. Although one usually thinks of metal as being a good conductor this problem is one in which the conductivity may be considered as very poor due to the short duration of the heat pulse.

An analysis of the behavior of solutions of equations of the general form

$$u_t = \epsilon\,[a(x)u_{xx} + b(x)u_x + c(x)u]$$

has been undertaken by the author and explicit formulas for such problems have been obtained through singular perturbation techniques. However, in the present paper we shall deal only with the diffusion equation $u_t = \epsilon u_{xx}$ due to space limitations. The behavior for this case is simpler than the general case but typical. At first only the Cauchy problem (infinite rod) will be analyzed. Later it will be shown how extensions to mixed initial-boundary problems are easily accomplished.

There has been some treatment of this type of problem in the literature — see, for example, references [1, 2, 3, 5]. All of these only develop the first order approximations, however, and require more stringent conditions on the data than we have found necessary. In particular the case where discontinuities arise between the boundary data and the initial data has not been analyzed. The present treatment is very direct in its approach and all of the approximations will be explicitly obtained. The precise effect of discontinuities in the data and its derivatives will be clear from the asymptotic representations obtained.

The results presented here are only partial and give an indication of the general approach. A full development for the more general case will be available in the author's thesis [6] which is currently being completed at the University of Delaware.

2. **Cauchy Problem for the Diffusion Equation.** Consider the following problem in the region $-\infty < x < \infty, 0 \leqq t < T$:

(1) $u_t = \epsilon u_{xx}$, for $t > 0$,

(2) $\text{limit}_{t \to 0} u(x, t) = \phi(x)$, wherever $\phi(x)$ is continuous,

(3) $|u(x, t)| \leqq M \exp[\alpha x^2]$, for $0 \leqq t < T$ and $-\infty < x < \infty$,

where M and α are positive constants.

The existence and uniqueness of the solutions of this type of problem are thoroughly discussed by A. Friedman in [4]. In the present discussion we shall be more concerned with the computational aspects of the problem. However, in passing, we should make a few remarks about those more fundamental questions: (a) The existence of a solution is guaranteed provided $4\epsilon\alpha T < 1$. (b) Condition (3) is sufficient to guarantee uniqueness. It is much weaker than the usual boundedness condition specified for such problems from physical reasoning. (c) Condition (2) should be replaced by a more general requirement if $\phi(x)$ is only locally integrable. However, we will consider only $\phi(x)$ which are continuous except at certain isolated points where it has well defined jumps. In such cases condition (2) is sufficient. (d) Condition (3) applies in particular to $\phi(x) = u(x, 0)$.

The solution of problem (1), (2), (3) can be written in the well known integral representation form

(4) $$u(x, t) = \int_{-\infty}^{\infty} F(x - y, \epsilon t)\phi(y)\, dy,$$
where $F(x, t) = (1/\sqrt{4\pi t}) \exp[-x^2/4t]$.

This integral is not always easy to evaluate explicitly or even numerically so we proceed with a singular perturbation analysis to obtain easily calculated solutions. We wish to emphasize here that the singular perturbation technique can be extended to more general equations where the fundamental solution is not known a priori.

3. **The Functions H_n, H_n^* and v_n.** In this section we introduce certain functions which will be convenient later in the discusssion.

Define the initial value functions $h_n(x)$ and h_n^* for $n = 0, 1, \cdots$

$$h_n(x) = \begin{cases} x^n/n!, & \text{for } x > 0 \\ 0, & \text{for } x < 0, \text{ and} \end{cases}$$
$$h_n^*(x) = \begin{cases} 0 & \text{for } x > 0 \\ x^n/n! & \text{for } x < 0. \end{cases}$$

The functions $H_n(x, t)$ and $H_n^*(x, t)$ are then defined as the (unique) solutions of $u_t = u_{xx}$ which satisfy the growth condition (3) and the respective initial conditions

$$H_n(x, 0) = h_n(x)$$
$$H_n^*(x, 0) = h_n^*(x)$$

Let the two auxiliary functions $E(x, t)$ and $F(x, t)$ be

$$E(x, t) = 1/2 \operatorname{erfc}(-x/\sqrt{4\pi t}),$$
$$F(x, t) = (1/\sqrt{4\pi t}) \exp[-x^2/4t],$$

where

$$\operatorname{erfc}(y) = (2/\sqrt{\pi}) \int_y^\infty \exp[-z^2]\, dz.$$

It is easy to show by induction that H_n satisfies the recursive formula

$$H_0 = E,$$
$$H_1 = xE + 2tF,$$
$$H_n = (1/n)(xH_{n-1} + 2tH_{n-2}), \quad \text{for } n \geqq 2.$$

Another useful formula for H_n is $H_n = (1/n!)[v_n E + 2u_n F]$, where u_n and v_n are polynomials in x and t defined by the recursive formulas

$$u_0 = 0, \qquad v_0 = 1,$$
$$u_1 = t, \qquad v_1 = x,$$
$$v_n = xv_{n-1} + 2(n-1)tv_{n-2},$$
$$u_n = xu_{n-1} + 2(n-1)tu_{n-2}.$$

Similarly, define E^* and F^* by

$$E^*(x, t) = E(-x, t)$$
$$F^*(x, t) = -F(x, t).$$

Then we can show

$$H_0^* = E^*,$$
$$H_1^* = xE^* + 2tF^*,$$
$$H_n^* = (1/n)[xH_{n-1}^* + 2tH_{n-2}^*], \text{ and}$$
$$H_n^* = (1/n!)[v_n E^* + 2u_n F^*].$$

The proof of all of these is routine so we omit it. The importance of the recursive relations is that they reduce all calculations to the evaluation of the well-known functions $\exp[-x^2]$ and $\operatorname{erfc}(x)$.

We note here that the polynomials $v_n(x, t)$ coincide with the heat polynomials discussed by Rosenbloom and Widder in [7]. Because $v_n(x, t)$ is a solution of the diffusion equation $u_t = u_{xx}$ and has initial values $v_n(x, 0) = x^n$, then

$$v_n(x, t) = n!\,[H_n(x, t) + H_n{}^*(x, t)]. \tag{5}$$

Let $L\phi = \phi_{xx}$. Then another convenient representation is

$$v_n(x, t) = \sum_{k=0}^{n'} L^k(x^n)t^k/k!, \tag{6}$$

where n' is the smallest integer not less than $n/2$. Note that n' can be replaced by any larger integer since $L^k(x^n) = 0$ for any $k > n/2$.

4. **Outer Solution.** The solution of (1), (2) and (3) is assumed to have the asymptotic representation

$$u(x, t) = \delta_0(\epsilon)u_0 + \delta_1(\epsilon)u_1 + \cdots, \text{ where}$$
$$\delta_0(\epsilon) = 1, \text{ and}$$
$$\delta_{k+1}(\epsilon) = o(\delta_k(\epsilon)) \quad \text{as } \epsilon \to 0^+, \text{ for } k = 0, 1, 2, \cdots$$

by standard procedures one easily can show that the only reasonable choice for the asymptotic sequence is $\delta_k(\epsilon) = \epsilon^k$. The equations for the u_k are then obtained by substituting into (1)

$$(u_0)_t = 0,$$
$$(u_k)_t = (u_{k-1})_{xx}, \qquad (k \geqq 1),$$

with initial conditions

$$u_0(x, 0) = \phi(x),$$
$$u_k(x, 0) = 0, \qquad (k \geqq 1).$$

these are easily solved when $\phi(x)$ is sufficiently differentiable,

$$u_k(x, t) = t^k L^k \phi(x)/k! \qquad (k \geqq 0).$$

The n-term outer expansion of solutions to (1), (2), (3) is therefore given by

$$u(x, t) = \sum_{k=0}^{n} (\epsilon t)^k L^k \phi(x)/k! + O((\epsilon t)^{n+1}), \tag{7}$$

where L^k is the operator L applied k times.

This representation is very advantageous for computations since it reduces the problem of finding u at a point (x_0, t) to the evaluation of ϕ and its derivatives at $x = x_0$. The error is of order $(\sqrt{\epsilon t})^{2n+1}$ provided ϕ has 2n + 1 continuous derivatives in a neighborhood $(x_0 - h, x_0 + h)$, where $h \gg \sqrt{\epsilon t}$. This claim is not difficult to prove using the integral representation for $u(x, t)$ and growth properties of $F(x, t)$. We shall not include a proof here.

In passing we note that for more general operators such as $Lu = a(x)u_{xx} + b(x)u_x + c(x)u$ the outer solution of $u_t = \epsilon Lu$ is given by the exact same formula, (7). In fact, this representation is a formal solution if $n = \infty$ and is a true solution whenever the series is defined and convergent for all x.

5. **Interior Layer.** In the usual singular perturbation problem the outer solution fails to satisfy some of the data specified in the original problem and an inner solution is derived to correct any discrepancies. In the present case, however, the outer solution satisfies the prescribed data, given by (2), so an inner solution is not required for the usual reason. This is a rather unique feature of the pure initial value problem under consideration and should not be expected in general. In contrast, if we were concerned with a mixed *BVP-IVP* problem, then the usual difficulties would arise.

There is, however, another source of singularities in the behavior of a perturbation solution, namely the presence of discontinuities in the prescribed data and its derivatives. It is apparent that this type of difficulty occurs with the representation (7) since any discontinuity in $\phi(x)$ or its derivatives are propagated into the solution domain along the sub-characteristics $x =$ constant. Solutions to the diffusion equation are known to be infinitely differentiable except at the boundaries, but (7) does not have that property. We are therefore led to the need for "interior layers" to correct the outer solution in the neighborhood of sub-characteristics. In general there can be many points at which $\phi(x)$ or its derivatives up to a given order do not exist. Our analysis will assume only one such point, namely $x = x_0$, but the results are easy to extend to the more general situation because of the linearity of solutions of (1).

There is another motive for studying the effect of discontinuities in the initial data for the Cauchy problem which is really the more important reason. In § 8 we shall show how mixed boundary-initial value problems can be transformed into Cauchy type problems with discontinuous data. The results we develop now will thus be directly applicable to that case and will lead to a proper understanding of the influence of the boundary data on the solution.

To proceed with an analysis of the Cauchy problem we assume that in some neighborhood $(x_0 - h, x_0 + h)$, $\phi(x)$ satisfies jump conditions in the form

$$\phi(x) = \begin{cases} \sum_{k=0}^{2n} (a_k/k!)(x - x_0)^k + R_{2n}, & \text{for } x > x_0 \\ \sum_{k=0}^{2n} (b_k/k!)(x - x_0)^k + R_{2n}^*, & \text{for } x < x_0, \end{cases} \tag{8}$$

where the Taylor remainders R_n and R_n^* are $O((x - x_0)^{2n+1})$.

To understand the behavior of $u(x, t)$ near to the sub-characteristic $x = x_0$, we introduce an inner variable of the form

$$\tilde{x} = (x - x_0)/\sqrt{\epsilon},$$

and an inner solution

$$U(\tilde{x}, t) = u(\sqrt{\epsilon}\tilde{x} + x_0, t), \tag{9}$$

which is assumed to have an asymptotic form

$$U(\tilde{x}, t) = U_0(\tilde{x}, t) + \delta_1(\epsilon)U_1(\tilde{x}, t) + \cdots, \tag{10}$$

where $\delta_1(\epsilon) = O(1)$, and

$$\delta_{k+1}(\epsilon) = o(\delta_k(\epsilon)), \qquad k \geqq 1.$$

Rewriting equation (1) in terms of $\tilde{x}$ gives the equation for U as

$$U_t = \epsilon(1/\sqrt{\epsilon})^2 U_{\tilde{x}\tilde{x}}. \tag{11}$$

Substitution of (10) into (11) leads to the following equation for U_0:

$$(U_0)_t = (U_0)_{\tilde{x}\tilde{x}}. \tag{12}$$

Initial conditions for $U(\tilde{x}, 0)$ follow from those for $u(x, t)$:

$$U(\tilde{x}, 0) = u(\sqrt{\epsilon}\tilde{x}, 0) = \phi(\sqrt{\epsilon}\tilde{x}).$$

Then from (8),

$$U(\tilde{x}, 0) = \begin{cases} \sum_{k=0}^{2n} (a_k/k!)(\sqrt{\epsilon}\tilde{x})^k + R_{2n}, & \text{for } \tilde{x} > 0 \\ \sum_{k=0}^{2n} (b_k/k!)(\sqrt{\epsilon}\tilde{x})^k + R_{2n}^*, & \text{for } \tilde{x} < 0. \end{cases} \tag{13}$$

This indicates that the proper choice for the asymptotic sequence in $\delta_k(\epsilon) = (\sqrt{\epsilon})^k$ and the asymptotic series for U is

$$U(\tilde{x}, t) = U_0(\tilde{x}, t) + \sqrt{\epsilon}U_1(\tilde{x}, t) + \epsilon U_2(\tilde{x}, t) + \cdots.$$

Substituting this expression into (11) and comparing with (13) we obtain equations and initial conditions for U_k:

$$(U_k)_t = (U_k)_{\tilde{x}\tilde{x}},$$

$$U_k(x, 0) = \begin{cases} (a_k/k!)\tilde{x}^k, & \text{for } \tilde{x} > 0 \\ (b_k/k!)\tilde{x}^k, & \text{for } \tilde{x} < 0. \end{cases}$$

Solving for U_k in terms of H_k and $H_k{}^*$ we have:

$$U_k(\tilde{x}, t) = a_k H_k(\tilde{x}, t) + b_k H_k{}^*(\tilde{x}, t), \text{ and}$$

$$U(\tilde{x}, t) = \sum_{k=0}^{2n} (\sqrt{\epsilon})^k [a_k H_k(\tilde{x}, t) + b_k H_k{}^*(\tilde{x}, t)] + O((\sqrt{\epsilon})^{2n+1}). \tag{14}$$

Relating u and U by (9) we then set $\bar{x} = x - x_0$ and obtain

$$\begin{aligned} u(x, t) &= U(\bar{x}/\sqrt{\epsilon}, t) \\ &= \sum_{k=0}^{2n} (\sqrt{\epsilon})^k [a_k H_k(\bar{x}/\sqrt{\epsilon}, t) + b_k H_k{}^*(\bar{x}/\sqrt{\epsilon}, t)] \\ &\quad + O((\sqrt{\epsilon})^{2n+1}), \text{ as } \epsilon \to 0. \end{aligned} \tag{15}$$

This representation has been derived only in a formal way, but it can be rigorously justified for $|x - x_0| < h$. We now wish to indicate how (15) can be written in the form of the "outer solution" (7) plus a correction term (which we call an "interior layer") to account for the discontinuities in $\phi(x)$ or its derivatives at $x = x_0$. Letting $d_k = a_k - b_k$, (15) can be rewritten

$$\begin{aligned} u(x, t) &= \sum_{k=0}^{2n} (\sqrt{\epsilon})^k a_k [H_k(\bar{x}/\sqrt{\epsilon}, t) + H_k{}^*(\bar{x}/\sqrt{\epsilon}, t)] \\ &\quad - \sum_{k=0}^{2n} (\sqrt{\epsilon})^k d_k H_k{}^*(\bar{x}/\sqrt{\epsilon}, t) + O((\sqrt{\epsilon})^{2n+1}) \\ &= \sum_{k=0}^{2n} (\sqrt{\epsilon})^k (a_k/k!)\, v_k(\bar{x}/\sqrt{\epsilon}, t) \\ &\quad - \sum_{k=0}^{2n} (\sqrt{\epsilon})^k d_k H_k{}^*(\bar{x}/\sqrt{\epsilon}, t) + O((\sqrt{\epsilon})^{2n+1}). \end{aligned}$$

But $v_k(\bar{x}/\sqrt{\epsilon}, t)$ is a solution to $u_t = \epsilon u_{xx}$, and similar to (6) we have

$$v_k(\bar{x}/\sqrt{\epsilon}, t) = \sum_{i=0}^{k'} (\epsilon L)^i (\bar{x}/\sqrt{\epsilon})^k t^i / i!.$$

Hence,

$$u(x, t) = \sum_{k=0}^{2n} (\sqrt{\epsilon})^k (a_k/k!) \left(\sum_{i=0}^{k'} (\epsilon L)^i (\bar{x}/\sqrt{\epsilon})^k t^i / i! \right)$$

$$- \sum_{k=0}^{2n} (\sqrt{\epsilon})^k d_k H_k^*(\bar{x}/\sqrt{\epsilon}, t) + O((\sqrt{\epsilon})^{2n+1}).$$

Because $k \leqq 2n$ implies $k' \leqq n$, k' can be replaced by n. Then reversing the order of the summation gives

$$u(x, t) = \sum_{i=0}^{n} (1/i!) t^i (\epsilon L)^i \left[\sum_{k=0}^{2n} (a_k/k!) \bar{x}^k \right]$$

$$- \sum_{k=0}^{2n} (\sqrt{\epsilon})^k d_k H_k^*(\bar{x}/\sqrt{\epsilon}, t) + O((\sqrt{\epsilon})^{2n+1})$$

$$= \sum_{i=0}^{n} (1/i!)(\epsilon t)^i L^i \left[\sum_{k=0}^{2n} (a_k/k!) \bar{x}^k \right]$$

$$- \sum_{k=0}^{2n} (\sqrt{\epsilon})^k d_k H_k^*(\bar{x}/\sqrt{\epsilon}, t) + O((\sqrt{\epsilon})^{2n+1}).$$

The expansion (13) of the initial value function can be used to simplify this for $x > x_0$:

$$u(x, t) = \sum_{i=0}^{n} (\epsilon t)^i L^i (\phi(x))/i!$$

$$(16) \qquad - \sum_{k=0}^{2n} d_k (\sqrt{\epsilon})^k H_k^*(\bar{x}/\sqrt{\epsilon}, t)$$

$$+ O((\sqrt{\epsilon})^{2n+1}$$

where $\bar{x} = x - x_0$.

By similar derivation the corresponding formula for $x < x_0$ can be obtained:

$$u(x,t) = \sum_{i=0}^{n} (\epsilon t)^i L^i(\phi(x))/i! + \sum_{k=0}^{2n} d_k(\sqrt{\epsilon})^k H_k(\bar{x}/\sqrt{\epsilon}, t) + O((\sqrt{\epsilon})^{2n+1}). \tag{17}$$

In this form it is apparent how the inner solution given by (16) for $x > x_0$ and by (17) for $x < x_0$ is just the outer solution plus a correction for the interior layer. An analysis of the functions H_n and H_n^* would show that $H_n(x,t)$ becomes negligible faster than any power of $(1/x)$ as $x \to -\infty$, and similarly, $H_n^*(x,t)$ becomes negligible as $x \to -\infty$. The correction terms in (16) and (17) are therefore negligible except in a neighborhood of the subcharacteristic $x = x_0$.

6. **Mixed Boundary–Initial Value Problems.** One of the techniques for solving mixed boundary–initial value problems is to convert the problem into an appropriate pure initial value problem for which the fundamental solution is known. The solution of the new problem is then shown to satisfy all of the conditions of the original problem. This approach is particularly useful in the present case since we have developed all of the necessary tools for solving the Cauchy problem.

Unfortunately, there does not seem to be any standard reference for this technique, and we do not have space here for discussing the matter. Therefore we shall only indicate the proper initial value problem which can be used to solve certain mixed boundary initial value problems. Greater detail will be included in [6] and will be submitted for publication in a separate paper.

The following list is valid for the equation $u_t = \epsilon u_{xx}$.

A. Semi-infinite domain, zero boundary condition.

Mixed BVP–IVP:	$u(x,0) = \phi(x)$,	$x > 0$,
	$u(0,t) = 0$,	$t > 0$.
Corresponding IVP:	$u(x,0) = \phi(x)$,	$x > 0$,
	$u(x,0) = -\phi(-x)$,	$x < 0$.

B. Semi-infinite domain, zero initial condition.

Mixed BVP-IVP:	$u(x,0) = 0$,	$x > 0$,
	$u(0,t) = h_n(t)$,	$t > 0$.
Corresponding IVP:	$u(x,0) = 2h_{2n}^*(x/\sqrt{\epsilon})$.	

C. Finite domain, zero boundary conditions.

Mixed BVP–IVP:

$$u(x,0) = h_n(x), \qquad 0 < x < x_0,$$
$$u(0,t) = 0, \qquad t > 0,$$
$$u(x_0,t) = 0, \qquad t > 0.$$

Corresponding IVP:

$$u(x,0) = h_n(x - 2kx_0) - |h_n{}^*(x - 2kx_0)|, \quad \text{for } (2k-1)x_0 < x < (2k+1)x_0.$$

D. Finite domain, one non-zero boundary condition.

Mixed BVP-IVP:

$$u(x,0) = 0, \qquad 0 < x < x_0,$$
$$u(0,t) = h_n(t), \qquad t > 0,$$
$$u(x_0,t) = 0, \qquad t > 0.$$

Corresponding IVP:

$$u(x,0) = 2\sum_{j=0}^{\infty} h_{2n}{}^*((x + 2_j x_0)/\sqrt{\epsilon}) - 2\sum_{k=1}^{\infty} h_{2n}((x - 2kx_0)/\sqrt{\epsilon}).$$

These correspondences combined with the theory developed in previous sections for the Cauchy problem allow us to solve the heat conduction problem in a finite rod explicitly when the data is given in the form of sufficiently smooth functions plus piecewise polynomials which can be discontinuous between pieces. The analysis developed in §§ 4 and 5 which assumes only one point where the data can be discontinuous can be directly applied to Examples A and B. By superposition the analysis can also be extended to problems where the data is discontinuous at a finite number of points. Furthermore the case of an infinite number of such points can be directly handled provided certain general growth conditions are satisfied by the data in particular asymptotic estimates can be developed for Examples C and D. A more detailed treatment can also be found in [6].

7. **Conclusions.** Basically what we have developed in this discussion is an alternative to the Fourier method for solving the diffusion equation. The present method, based on asymptotic analysis, is accurate for small ϵt and is particularly advantageous when any sort of discontinuities are present in the initial and boundary data. In general very few terms are needed to give accurate estimates of the solution. To contrast this with the Fourier approach one should note how many terms are required to resolve a discontinuous function into sines and cosines with reasonable accuracy. Although the higher frequency modes tend to cancel out and become insignificant with time

this is not helpful in describing the early development of the solution.

In our opinion the present method is a far more natural approach to diffusion problems when steep gradients are present. It also has the advantage of providing formulae rather than numbers for describing the physical behavior.

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