LBNL-40868
UC-405
Preprint

ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

Conditions for Thermal Explosion in a Flowing Gas: Numerical Methods

Anton Kast

Computing Sciences Directorate
Mathematics Department

September 1997

To be submitted
for publication

REFERENCE COPY
Does Not
Circulate
Bldg. 50 Library - Ref.
Lawrence Berkeley National Laboratory
Copy 1
LBNL-40868

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

LBNL-40868

CONDITIONS FOR THERMAL EXPLOSION IN A FLOWING GAS: NUMERICAL METHODS*

Anton Kast

Mathematics Department
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

September 1997

*This work was supported in part by the Applied Mathematical Sciences Subprogram of the Office of Energy Research, U.S. Department of Energy, under Contract DE-AC03-76SF00098, and in part by the National Science Foundation under Grant DMS94-14631.

Conditions for Thermal Explosion in a Flowing Gas: Numerical Methods *

Anton Kast
Mathematics Department
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

Abstract

In the classical theory of thermal explosions, the condition for explosion to occur is that a particular nonlinear elliptic partial differential equation must have no solutions. In a recent paper, combustion in a cylindrical pipe with flowing reactant was studied, and it was claimed that the answer to the existence question in that case depended on the length of the pipe. In this paper, we describe the numerical methods used to determine existence and nonexistence of solutions to the differential equations in that case. We also describe scaling laws in this system which have been shown numerically but not yet understood theoretically.

*Supported in part by the Applied Mathematical Sciences subprogram of the Office of Energy Research, U.S. Department of Energy, under contract DE–AC03–76–SF00098, and in part by the National Science Foundation under grant DMS94–14631.

1 Introduction

The classical theory of thermal explosions, as presented in [1], considers the flow of heat produced in chemical reactions. It describes the conditions for balance between the production of heat in reactions and the diffusion of heat to the boundaries of the reactant. An explosion is then expected to occur when no such balance is possible, in the sense that the equation of balance has no solutions. If one wants to predict whether reactions in a container will proceed smoothly or abruptly, one must therefore determine whether a particular nonlinear partial differential equation with some particular boundary conditions does or does not have solutions.

Confronted with a nonlinear boundary value problem, we may be tempted to use a computer to find solutions. If the computer finds a solution then we know something, but if the computer fails to find a solution then it is not clear what we can infer. To use a computer, we must replace the differential equations with some convergent, discretized system of (generally transcendental) equations, and it is quite possible for solutions to such systems to be overlooked by any numerical scheme. To answer questions about explosions, we must figure out how to use a computer to claim that a transcendental system of equations has no solutions.

In this paper, we study the particular nonlinear PDEs that have arisen recently in a study of axisymmetric reacting flow in a cylindrical pipe [2]. These equations present a tractable existence question because solutions are easy to find for some values of physical parameters and because the existence region in the parameter space may be presumed to have a simple, smooth boundary. We determine the existence-nonexistence curve in this parameter space by first constructing solutions on the existence side and then approaching the boundary in small increments. Thus, we may always be sure that if a solution exists, we know almost exactly what it looks like.

2 Formulation of the Problem

We assume that the chemical reaction is proceeding in a container and that the density of the reactant is constant throughout the container. The temperature T as a function of position is described by the heat equation

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T + \frac{Q}{c} W(T) \tag{1}$$

where κ is the thermal diffusivity of the reacting matter, Q is the reactant's heat of reaction per unit mass, c is its specific heat capacity, and $W(T)$ is its temperature-dependent reaction rate. The temperature can settle down to a steady distribution if there is a function T consistent with the boundary

conditions such that the time derivative in (1) is zero.

Following [2], we consider combustion in a cylindrical vessel with reactant flowing along the cylinder. We use cylindrical coordinates and assume axisymmetry, with r being the radius and z being the distance along the pipe from the point where reactions begin. We take the radius of the pipe to be r_0. The cylinder walls enforce a constant temperature, $T(r_0, z) = T(r, 0) = T_0$ at the boundaries.

We proceed to make the classical assumptions about chemical reactions: we assume $W(T)$ has the exponential form given by an Arrhenius law,

$$W(T) = \sigma(T)e^{-E/RT} \tag{2}$$

with $\sigma(T)$ something close to a power law in T, E the activation energy of the chemical reaction and R the universal gas constant; and we assume that the activation energy E in this law is large so that we may make the Frank-Kamenetskii transformation [3] (see [1]) where we linearize the exponent near T_0. This means that we approximate,

$$W(T) \approx \sigma(T_0)e^{-E/RT_0}e^{\frac{E}{RT_0^2}(T-T_0)}. \tag{3}$$

The advection of reactant adds an advective term $v(r)\partial_z T(r, z)$ to (1) where $v(r)$ is the local axial velocity. According to the familiar solution to

the Navier-Stokes equation in a cylinder, $v(r) = 2\overline{v}[1-(r/r_0)^2]$ where $\overline{v}$, the average of $v(r)$ over the cylinder cross-section, parameterizes the flow. We assume that we may neglect diffusion in the axial direction compared to the advection.

Changing (1) to dimensionless variables, adding the advective term and setting the time derivative to zero, the steady-state equation for temperature in this system is

$$\frac{1}{\rho}\partial_\rho\left(\rho\partial_\rho u\right) + \lambda^2 e^u = (1-\rho^2)\partial_\zeta u \tag{4}$$

where $u = (T-T_0)E/RT_0^2$ is the rescaled temperature, $\rho = r/r_0$ is a dimensionless pipe radius, $\zeta = z(\kappa/2\overline{v}r_0^2)$ is a dimensionless longitudinal coordinate, and $\lambda = r_0/\ell$ is the pipe radius r_0 normalized by the characteristic length,

$$\ell = \left[\frac{\kappa c R T_0^2 e^{E/RT_0}}{Q\sigma(T_0)E}\right]^{1/2}. \tag{5}$$

In the new variables, the domain of computation is $0 < \rho < 1$ and $0 < \zeta$. At $\rho = 1$ and at $\zeta = 0$ we require $u = 0$. At $\rho = 0$, on the axis, we assume that the heat flux must go to zero. The boundary conditions on (4) are therefore

$$u(\rho,0) = 0, \quad u(1,\zeta) = 0, \quad \lim_{\rho\to 0}\left[\rho\partial_\rho u(\rho,\zeta)\right] = 0. \tag{6}$$

The limiting flux condition is simply the condition that $\partial_\rho u(0,\zeta) = 0$. To see that this is so, we may multiply both sides of (4) by ρ and integrate:

$$\rho\partial_\rho = \int^\rho \left[(1-r^2)\partial_\zeta u - \lambda^2 e^u\right] r\,dr. \tag{7}$$

Near $\rho = 0$, assuming $u(0,\zeta)$ and $\partial_\zeta u(0,\zeta)$ are finite, this integral may be approximately evaluated to yield

$$\partial_\rho u(\rho,\zeta) = \frac{1}{2}\rho\left[\partial_\zeta u(0,\zeta) - \lambda^2 e^{u(0,\zeta)}\right] + \frac{C}{\rho} + O(\rho^2) \tag{8}$$

where C is a constant of integration. This expression shows that either u diverges logarithmically at $\rho = 0$ or $\partial_\rho u(0,\zeta) = 0$. Thus the limit condition in (6) is equivalent to the constraints that $C = 0$, that $u(0,\zeta)$ is finite, or that $\partial_\rho u(0,\zeta) = 0$.

The parabolic equation (4) together with boundary conditions (6) specify the conditions for thermal explosion in this geometry. Given the velocity profile $V(\rho)$, the system has only one parameter, λ, and it is proportional to the pipe radius. The boundary condition at $\zeta = 0$ has a stabilizing effect and ensures that for any λ, solutions may be found up to some positive ζ. It is possible however that for some λ, the parabolic equation may not be integrated beyond some point $\zeta_0(\lambda)$. This critical length, dependent on λ, is the principal result presented in [2]. In dimensionless variables, it is the

maximum length of pipe in which reactions can occur without explosion.

After studying this laminar case, the authors of [2] proceeded to generalize (4) to the case that the reactant is turbulent. They replaced $V(\rho)$ by a mean velocity profile obtained from scaling analysis, and they similarly replaced the thermal diffusivity κ with a radius-dependent turbulent effective diffusivity. The resulting equation, in new dimensionless variables, was

$$\frac{1}{\rho}\partial_\rho\left[\rho^2(1-\rho)^{1-\alpha}\partial_\rho u\right] + \lambda^2 e^u = (1-\rho)^\alpha \partial_\zeta u \tag{9}$$

where $\alpha = 3/2\log(Re)$ is determined by the Reynolds number Re of the turbulent flow, and the new boundary conditions were

$$u(\rho,0) = 0, \quad u(1,\zeta) = 0, \quad \lim_{\rho\to 0}\left[\rho^2\partial_\rho u(\rho,\zeta)\right] = 0. \tag{10}$$

The new limiting flux condition is also equivalent to a constraint on $\partial_\rho u$. Performing the same asymptotic calculation near $\rho = 0$ on (9) as we did on (4), we see that

$$\partial_\rho u(\rho,\zeta) = \frac{1}{2}\left[\partial_\zeta u(0,\zeta) - \lambda^2 e^{u(0,\zeta)}\right] + \frac{C}{\rho^2} + O(\rho) \tag{11}$$

where C is a new constant of integration. Now we see that in the turbulent case, either u diverges like ρ^{-1} at $\rho = 0$ or a certain relationship exists at $\rho = 0$ between u, $\partial_\rho u$ and $\partial_\zeta u$. Thus the limit condition in (10) is equivalent

to the constraints that $C = 0$, that $u(0, \zeta)$ is finite, or that

$$\partial_\rho u(0, \zeta) = \frac{1}{2}\left[\partial_\zeta u(0, \zeta) - \lambda^2 e^{u(0,\zeta)}\right]. \tag{12}$$

In subsequent sections we will show how to compute the critical pipe length, $\zeta_0(\lambda)$, for the laminar equation (4), (6) and for the turbulent case (9), (10) by attempting to solve finite difference formulas for these and detecting when the computational domain precludes solutions.

3 Laminar Case

We want to compute solutions $u(\rho, \zeta)$ to the differential equation,

$$\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial u}{\partial \rho}\right) + \lambda^2 e^u - (1 - \rho^2)\frac{\partial u}{\partial \zeta} = 0 \tag{13}$$

with boundary conditions

$$u(\rho, 0) = 0, \quad u(1, \zeta) = 0, \quad \frac{\partial u}{\partial \rho}(0, \zeta) = 0, \tag{14}$$

in the domain $0 < \rho < 1$, $0 < \zeta$ for a given positive number λ. We expect that for some values of λ, solutions will only exist when ζ is less than some critical value, $0 < \zeta < \zeta_0(\lambda)$. In such cases we would like to determine the function $\zeta_0(\lambda)$.

3.1 Numerical scheme

Since it is inconvenient to vary the computational domain, we suppose that some number ζ_0 has already been proposed. Then we may change variables from ζ to $z = \zeta/\zeta_0$, so that (13) becomes

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial u}{\partial\rho}\right) + \lambda^2 e^u - \frac{1}{\zeta_0}(1-\rho^2)\frac{\partial u}{\partial z} = 0 \tag{15}$$

and (14) becomes

$$u(\rho,0) = 0, \quad u(1,z) = 0, \quad \frac{\partial u}{\partial\rho}(0,z) = 0, \tag{16}$$

with domain $0 < \rho < 1$, $0 < z < 1$. Both ζ_0 and λ now appear as parameters, and the question may be recast: For what values of the parameters does a solution exist on this fixed domain? We would like to determine the boundary of the existence region in the λ-ζ_0 plane.

Our strategy to determine this boundary is as follows. We will discretize the equations (15), (16) to get a system of transcendental equations for u at grid points. We will then attempt to solve the system using Newton's method. If Newton's method converges for a particular pair λ, ζ_0 then we say that the pair is inside the existence region and if the method does not converge then we say the pair is outside.

Newton's method is iterative, and an initial condition for iteration must be chosen. If this initial condition is close to an actual solution, then the method is rapidly convergent. If the initial condition is not close to an actual solution, then the method may fail to converge even when a solution exists. To pick initial conditions, we first presume that for any λ, a solution can be found if ζ_0 is sufficiently small. We pick λ, compute a solution for some ζ_0 sufficiently small that the solver converges, then increment ζ_0 and solve again starting from the initial condition given by the preceding solution. When ζ_0 becomes so large that the solver fails to converge, we say that we have crossed the existence boundary.

We introduce an $M \times N$ computational grid with discrete coordinates

$$\begin{aligned} r_i &= (i+1)/M, \quad i = 0, \ldots, M-1 \\ z_j &= (j+1)/N, \quad j = 0, \ldots, N-1 \end{aligned} \tag{17}$$

and discretized dependent variables

$$u_{i,j} \equiv u(\rho_i, z_j). \tag{18}$$

The operators appearing in equation (15) have discrete counterparts determined by finite differencing. We define a forwards ρ-derivative,

$$D_\rho^+(u)_{i,j} = \begin{cases} M\left(u_{i+1,j} - u_{i,j}\right), & i = 0 \ldots M-2, \quad j = 0 \ldots N-1 \\ M\left(u_{M-1,j} - u_{M-2,j}\right), & i = M-1, \quad j = 0 \ldots N-1 \end{cases} \tag{19}$$

a backwards ρ-derivative,

$$D_\rho^-(u)_{i,j} = \begin{cases} M\left(u_{1,j} - u_{0,j}\right), & i = 0, \quad j = 0 \ldots N-1 \\ M\left(u_{i,j} - u_{i-1,j}\right), & i = 1 \ldots M-1, \quad j = 0 \ldots N-1 \end{cases} \tag{20}$$

a backwards z-derivative,

$$D_z^-(u)_{i,j} = \begin{cases} N\left(u_{i,1} - u_{i,0}\right), & i = 0 \ldots M-1, \quad j = 0 \\ N\left(u_{i,j} - u_{i,j-1}\right), & i = 0 \ldots M-1, \quad j = 1 \ldots N-1 \end{cases} \tag{21}$$

and multiplication by ρ,

$$R(u)_{i,j} = \rho_i \times u_{i,j}. \tag{22}$$

(We use forward- and backward-differences to avoid decoupling of even and odd grid points. By using a backwards z-derivative only, we ensure unconditional stability in the sense of diffusive initial value problems.)

The equation (15) may be expressed in discretized form as

$$\left[L(u) + \lambda^2 e^u\right]_{i,j} = 0 \tag{23}$$

where L is a linear operator defined by composition of the elementary discrete operators,

$$L = R^{-1} D_\rho^+ R D_\rho^- - \frac{1}{\zeta_0}(I - R^2) D_z^- \tag{24}$$

(I denotes the identity operator) and e^u is the operator of local exponentiation,

$$(e^u)_{i,j} = e^{u_{i,j}}. \tag{25}$$

We want the discretized equations (23) to apply in the bulk of the computational domain, but at its boundary we want the boundary conditions to hold. Referring to equations (16), in the discrete variables we want to enforce

$$\begin{aligned} u_{i,0} &= 0, \quad i = 0 \ldots M-1 \\ u_{M-1,j} &= 0, \quad j = 0 \ldots N-1 \\ u_{1,j} - u_{0,j} &= 0, \quad j = 0 \ldots N-1. \end{aligned} \tag{26}$$

The actual system of MN transcendental equations that we will attempt solve using Newton's method is therefore

$$D(u)_{i,j} = 0 \tag{27}$$

where the operator $D(u)$ is defined to be

$$D(u)_{i,j} = \begin{cases} L(u)_{i,j} + \lambda^2 (e^u)_{i,j} & i = 1 \ldots M-2 \quad j = 1 \ldots N-1 \\ u_{i,0} & i = 0 \ldots M-1 \quad j = 0 \\ u_{M-1,j} & i = M-1 \quad j = 0 \ldots N-1 \\ u_{1,j} - u_{0,j} & i = 0 \quad j = 0 \ldots N-1. \end{cases} \tag{28}$$

This system of equations is convergent to the differential equation (15) with boundary conditions (16). If we find a sequence of solutions to (27) which is convergent as $M, N \to \infty$, then we have found an approximate solution to the differential equation (15) and we say that a solution to (15), (16) exists for the values of λ, ζ_0 used.

Newton's method may be applied directly to the system of transcendental equations (27). All that is needed is a formula for the matrix of derivatives,

$$\frac{\partial D(u)_{i,j}}{\partial u_{i',j'}}. \tag{29}$$

Then if we have an intermediate guess $u^{(n)}$ for u at step n of the method we can use the first-order Taylor series approximation

$$D(u^{(n)})_{i,j} + \sum_{i'=0}^{M-1} \sum_{j'=0}^{N-1} \left(u^{(n+1)} - u^{(n)}\right)_{i',j'} \left.\frac{\partial D(u)_{i,j}}{\partial u_{i',j'}}\right|_{u=u^{(n)}} = 0 \qquad (30)$$

to determine an improved guess $u^{(n+1)}$ implicitly. The needed matrix (29) is readily determined away from boundaries to be

$$\frac{\partial D(u)_{i,j}}{\partial u_{i',j'}} = L_{(ij),(i'j')} + e^{u_{i,j}} \delta_{(ij),(i'j')}. \qquad (31)$$

At boundaries the matrix is trivial to compute by differentiation of the boundary expressions shown in equation (28).

3.2 How to tell if Newton's method has converged

The iteration implied in (30) may be continued indefinitely. A condition is required for distinguishing when iterations have converged and when they are never going to converge.

At each step of iteration, we examined the maximum value over all i and j of the absolute value of $D(u)_{i,j}$ in equation (28). We called this maximum the numerical error of the current guess. If this error was less than 10^{-12}, we said that iterations had converged.

Experience indicated that if error was not monotonically decreasing, then it would never approach such a small value, even after hundreds of iterations.

For all parameter values, at least ten iterations of Newton's method were performed starting from a known nearby solution. If after this time growth in the error was observed, or if the error exceeded the maximum value of the computer's double precision arithmetic, then it was concluded that iterations would never converge.

3.3 Results

When $0 < \lambda < 2$, our method identifies convergent solutions for all values of ζ_0 tested. When $\lambda > 2$, our method identifies convergent solutions for all values of ζ_0 less than a critical value $\zeta_0(\lambda)$. To identify $\zeta_0(\lambda)$ for a given value of λ, we first find a large ζ_0 for which we can observe Newton's method to converge. We then increment ζ_0 by a small amount and reapply Newton's method using the converged solution from the previous value of ζ_0 as our initial guess. Eventually, ζ_0 can no longer be incremented without preventing the solver from converging. The highest convergent value of ζ_0 is $\zeta_0(\lambda)$.

Figure 1 shows a graph of $\zeta_0(\lambda)$ calculated with $M = N = 20$. Figure 2 shows a typical solution from a particular point in the $\lambda - \zeta_0$ plane. The salient features are the divergence of $\zeta_0(\lambda)$ on the left,

$$\lim_{\lambda^2 \to 2_+} \zeta_0(\lambda) = \infty \tag{32}$$

and the asymptotic power law behavior of $\zeta_0(\lambda)$ as $\lambda \to \infty$, determined by least-squares fitting to be

$$\zeta_0(\lambda) \sim (\lambda^2)^{-1.38} \qquad (\lambda \gg 1). \tag{33}$$

4 Turbulent Case

In developed turbulence, instead of (15) the equation becomes

$$\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho^2(1-\rho)^{1-\alpha}\frac{\partial u}{\partial \rho}\right) + \lambda^2 e^u - \frac{1}{\zeta_0}(1-\rho)^{\alpha}\frac{\partial u}{\partial z} = 0 \tag{34}$$

where $\alpha = 3/2\log(Re)$ and Re is the Reynolds number. The computational domain is the same as in (15). The boundary conditions are

$$u(\rho, 0) = 0, \quad u(1, z) = 0, \quad u(0, z) = (\text{finite}). \tag{35}$$

The unusual boundary condition on $u(0, z)$ could equivalently be that the heat flux vanishes at $\rho = 0$, that equation (12) holds, or that the constant of integration C in Section (11) is chosen to be zero.

4.1 Numerical scheme

To reduce numerical error near $\rho = 1$, where u has infinite derivatives, we change variables to $r = (1-\rho)^{\alpha}$. The equation in the new variable is

$$\frac{\alpha^2}{1-r^{1/\alpha}} r^{\frac{\alpha-1}{\alpha}} \frac{\partial}{\partial r}\left((1-r^{1/\alpha})^2 \frac{\partial u}{\partial r}\right) + \lambda^2 e^u - r\frac{\partial u}{\partial z} = 0 \tag{36}$$

and the new boundary conditions are

$$u(r,0) = 0$$

$$u(0,z) = 0 \quad . \tag{37}$$

$$u(1,z) = \text{(finite)}$$

We may further reduce numerical error by performing the outer differentiation in (36) and cancelling singular terms:

$$\alpha^2 r(r^{-1/\alpha} - 1)\frac{\partial^2 u}{\partial r^2} - 2\alpha\frac{\partial u}{\partial r} + \lambda^2 e^u - r\frac{\partial u}{\partial z} = 0. \tag{38}$$

Equation (38) with boundary conditions (37) offers the problem in a computationally tractable form. We proceed to solve this system numerically.

With the same discretization as in the preceding section, and using the same or analogous operators D_r^+, D_r^-, D_z^-, R (now multiplication by r instead of ρ), and e^u, we define our discretized system of equations to be $D(u)_{i,j} = 0$ where

$$D(u)_{i,j} = \begin{cases} L(u)_{i,j} + \lambda^2(e^u)_{i,j} & i = 1\ldots M-2 \quad j = 1\ldots N-1 \\ u_{i,0} & i = 0\ldots M-1 \quad j = 0 \\ u_{M-1,j} & i = M-1 \quad j = 0\ldots N-1 \end{cases} \tag{39}$$

and where now, in the turbulent case, the linear part is

$$L = \alpha^2 R(R^{-1/\alpha} - I)D_r^+ D_r^- - 2\alpha D_r^- - \frac{1}{\zeta_0} R D_z^-. \tag{40}$$

The needed matrix of derivatives may be determined as in the laminar case.

4.2 How to tell if Newton's method has converged

As in Subsection (3.2), we may define the error of a guessed solution by the maximum over i and j of the absolute value of $D(u)_{i,j}$. However, we can not determine convergence of iterations by using a small threshold value for this error. Unlike the laminar case, near $\rho = 1$ the turbulent solutions become steep like $(1-\rho)^{\alpha}$. The value of the turbulent $D(u)$ depends on cancellations between very large derivatives and very small coefficients. Roundoff error limits how small the error can be, in a way that depends on the Reynolds number through α. For the Reynolds numbers studied, using the double precision arithmetic of our Sun Ultra 2, roundoff error implied minimum errors in $D(u)$ of order 10^{-8}. The minimum error can be arbitrarily large if the Reynolds number is large enough.

Convergence could be defined by the approach of the error to the roundoff-determined minimum error. Rather than dealing with the subtleties of roundoff however, we chose to define convergence in terms of the step size of the Newton iterates. The *change* in the guessed solution at the nth iteration, $|u^{n-1} - u^n|$, has a maximum over i, j also. If this number was less than 10^{-12} then we said that the method had converged for the turbulent case. We similarly defined nonconvergence as in the laminar case but referring to this

step size rather than the original error value.

The threatening possibility is that this convergence criterion could mistake an extremely tight limit cycle for an actual zero of the functional (39). We see no way that this difficulty can be surmounted at the level of principle. Any guessed solution, whether obtained by Newton's method, simulated annealing, or any other procedure, would have to be plugged into the discretized equations and the same problem of roundoff error would enter.

We did verify however that the actual error of solutions was of the order of the roundoff limit when the new convergence criterion was satisfied.

4.3 Results

Figure 3 shows graphs of $\zeta_0(\lambda)$ for equation (34), (35) calculated with $M = N = 20$. Figure 4 shows a typical solution for a particular point in the $\lambda - \zeta_0$ plane and at $Re = 10^6$. At each value of the Reynolds number, there is a critical value of λ where $\zeta_0(\lambda)$ diverges. Figure 5 shows these critical values versus Reynolds number.

Figure 3 shows a power law behavior of $\zeta_0(\lambda)$ for all λ right of the critical value. This power law was determined by least-squares fitting to be

$$\zeta_0(\lambda) \sim (\lambda^2)^{-1.11} \qquad (\lambda \gg 1). \tag{41}$$

5 Conclusions

We have shown how an existence question for solutions of a nonlinear partial differential equation may be resolved numerically. Starting from points in the parameters space where a solution could be found, we probed neighboring parts of parameter space until a boundary of the existence region could be identified.

Considering laminar and turbulent flow in a pipe, we identified critical pipe lengths for thermal explosion to occur. The critical lengths depended on the pipe radius. We found asymptotic power-law dependence of the critical lengths on radius. We found asymptotically universal, Reynolds number-independent behavior for turbulent flow when the radius was large.

6 Acknowledgements

The author thanks Professors A.J. Chorin and G.I. Barenblatt and Dr. R. Kupferman for many helpful conversations.

References

[1] Ya.B. Zeldovich, G.I. Barenblatt, V.B. Librovich, and G.M. Makhviladze, *The Mathematical Theory of Combustion and Explosions*, Consultants

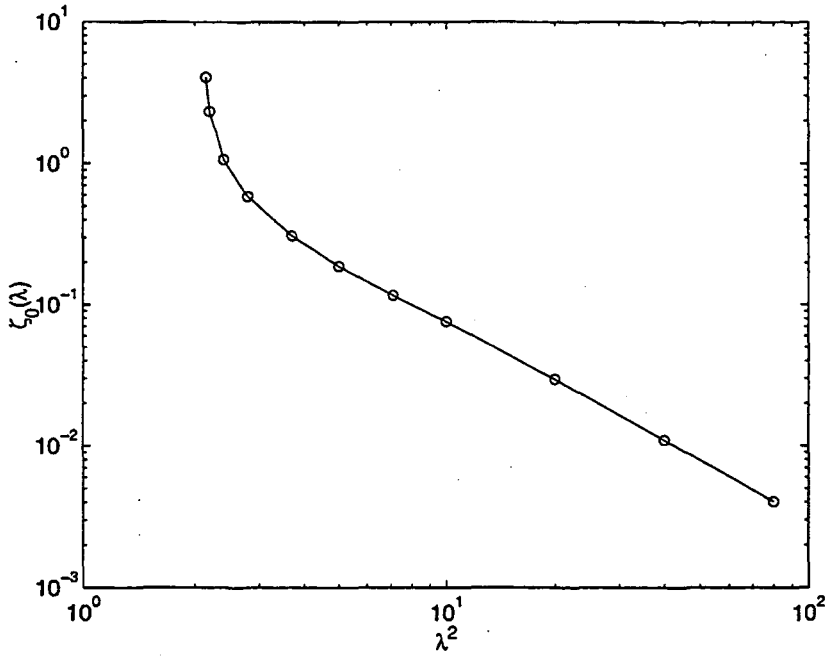

Figure 1: A graph of the boundary of the existence region for solutions of equations (15), (16). Solutions exist below the curve.

Bureau, New York, London, 1985.

[2] G.I. Barenblatt, A.J. Chorin, A. Kast, *Influence of flow of reactant on conditions for thermal explosion*, submitted to Proc. Nat. Acad Sc.

[3] D.A. Frank-Kamenetskii, *Zh. Fiz. Khim.*, 13 (1939), 738.

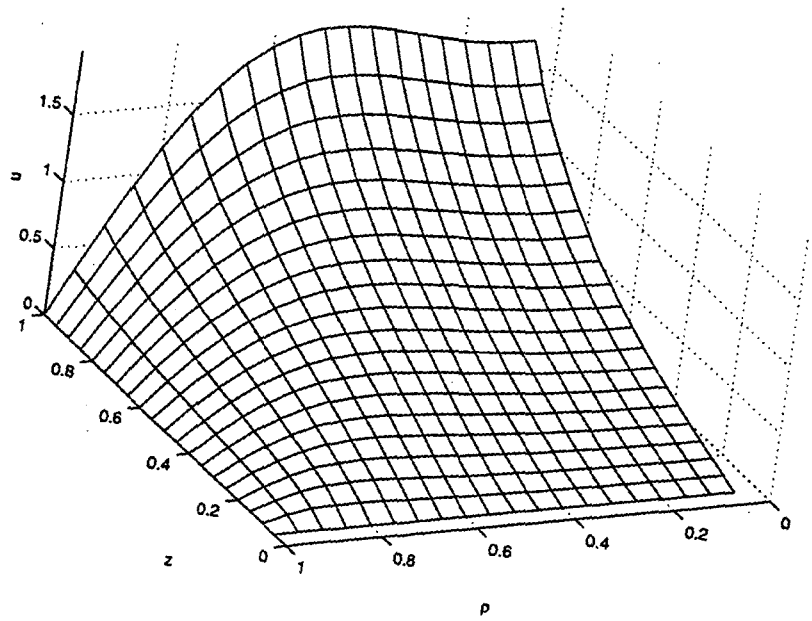

Figure 2: Solution to the equations (15), (16) for $\lambda^2 = 10$ and $\zeta_0 = .07$.

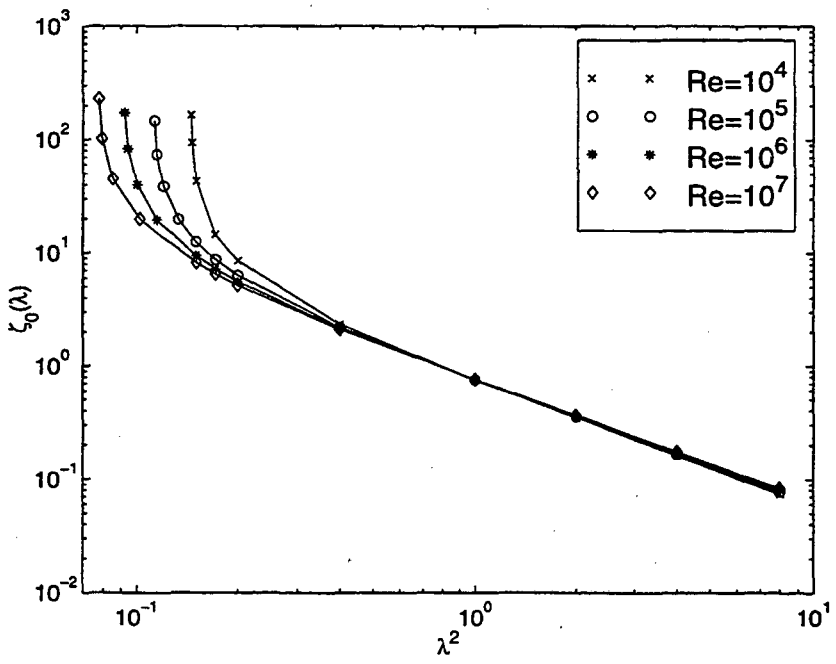

Figure 3: Existence boundaries for the turbulent equation at a variety of Reynolds numbers.

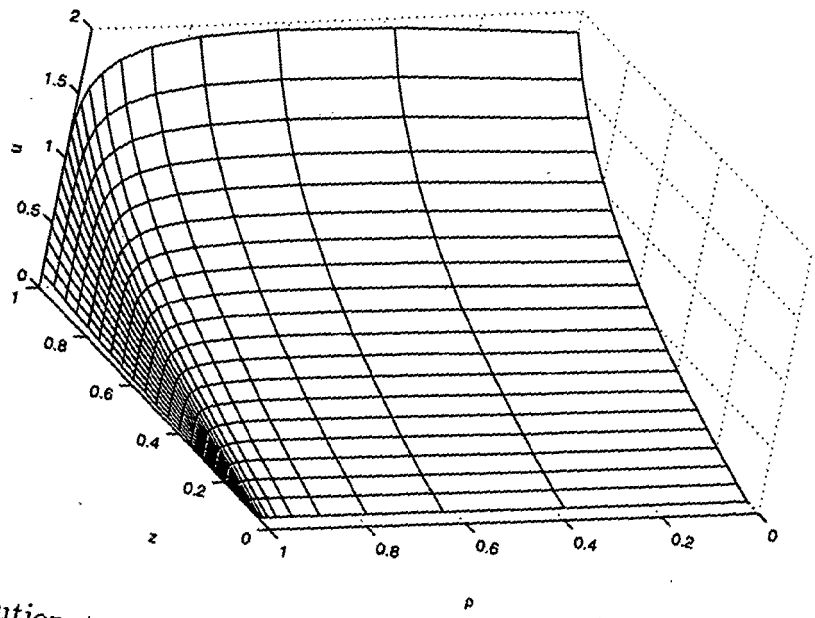

Figure 4: Solution to the equations (34), (35) for $\lambda^2 = 1$, $\zeta_0 = .8$, and $Re = 10^6$.

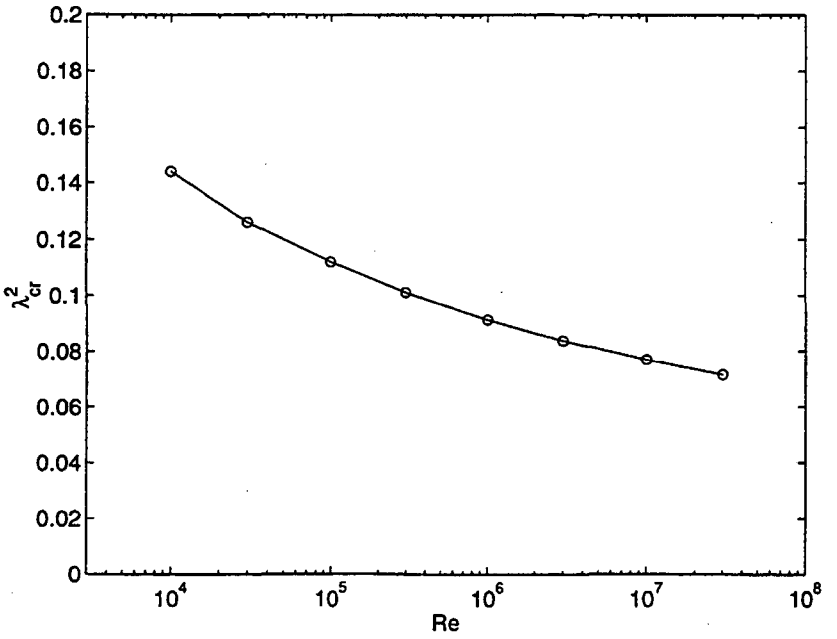

Figure 5: Critical values of λ versus Reynolds number.

Ernest Orlando Lawrence Berkeley National Laboratory
One Cyclotron Road | Berkeley, California 94720

Prepared for the U.S. Department of Energy under Contract No. DE-AC03-76SF00098