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RECENT PROGRESS IN THE THEORY OF THERMAL INSTABILITY USING Mathematica

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Abstract

The aim of this paper is to present our progress in the theory of thermal instability facilitated by the use of the *Mathematica*[1]. This progress enables the exact numerical solution of long-standing unsolved problems in the linear theory of thermal convection in horizontal layers and spherical shells of Newtonian or viscoelastic fluids in the presence or absence of rotation and/or magnetic field.

In the first part of the paper, our recent direct method for solving the several characteristic value problems arising in the linear theory of buoyancy-driven thermal convection in a horizontal layer of fluid heated from below in the absence or presence of rotation and/or magnetic field is presented. Necessary and sufficient conditions for the existence of non-trivial solutions of several characteristic value problems are derived in the general case, and then the method is favourably applied to study the thermal instability of a layer confined by any type of boundaries (Bénard problem). The method is rigorous, simple to apply, applicable to any type of boundaries: free, rigid , mixed, perfectly conducting or non-conducting, and moreover, it is easily implemented using *Mathematica*. Some unsolved convection problems with rotation and

magnetic field acting simultaneously can be tackled for the first time using this method.

As a second illustration of our progress, the thermal instability of an incompressible fluid sphere heated within and in equilibrium under its own gravitation is considered. Using the finite difference method in conjunction with *Mathematica*, a simple two step algorithm is derived to solve the eigenvalue problem which describes the onset of convection. It is shown that with literally only a few lines of code we can obtain with ease accurate results comparable with the best currently available results obtained by very tedious laborious "exact" techniques or the most incisive "approximate" variational techniques. While this analysis is limited to the case of thermal instability in a homogeneous sphere, the method can be readily applied to the treatment of convection in spherical shells.

1 The Bénard problem

Consider a horizontal layer of fluid in which an adverse temperature gradient is maintained by heating the underside. Since the fluid at the bottom is less dense than the fluid at the top, there will be a tendency on the part of the fluid to redistribute itself. However this tendency will be inhibited by its viscosity and we expect that the adverse temperature gradient must exceed a certain value before the instability can manifest itself.

Rayleigh established the stability or instability of a layer of fluid heated from below is dependent on the value of the non-dimensional parameter (*Rayleigh number*)

$$R = \frac{g\alpha\beta}{\kappa\nu} d^4, \tag{1}$$

where g denotes the acceleration due to gravity, d the depth of the layer, β the uniform adverse temperature gradient which is maintained, and α, κ,and ν are the coefficients of volume expansion, thermometric conductivity, and kinematic viscosity, respectively. The instability sets in when R exceeds a certain critical value R_c. The principal theoretical objective is to determine R_c.

Using the normal mode analysis, the linear equations governing the marginal state for the onset of stationary convection are [2]

$$(D^2 - a^2)^2 W = Ra^2 \Theta \tag{2}$$

$$(D^2 - a^2)\Theta = -W \tag{3}$$

subject to the boundary conditions for the three boundary types

(A) two free boundaries

$$W = D^2 W = \Theta = 0, \;\; z = 0, 1 \tag{4}$$

(B) two rigid boundaries

$$W = DW = \Theta = 0, \;\; z = 0, 1 \tag{5}$$

(C) one free and one rigid boundary

$$W = DW = \Theta = 0, \;\; z = 0$$

$$W = D^2 W = \Theta = 0, \;\; z = 1 \tag{6}$$

where $D = d/dz$, W and Θ are the perturbations in the z-components of velocity and temperature respectively, and a is the wave number.

Let $\mathbf{x}(z)$ be a real 6-dimensional vector function of z and $x_1(z) = W(z)$, $x_5(z) = \Theta(z)$. Equations (2) and (3) are equivalent to the 6th order system of linear first order differential equations.

$$x_i' = x_{i+1} \quad i = 1, 2, 3, 5 \tag{7}$$

$$x_4' = -a^4 x_1 + 2a^2 x_3 + Ra^2 x_5 \tag{8}$$

$$x_6' = -x_1 + a^2 x_5 \tag{9}$$

where $x_i' = dx_i/dz$. The boundary conditions defining the three different types of boundaries are:

(A)

$$x_1 = x_3 = x_5, \quad z = 0, 1 \tag{10}$$

(B)

$$x_1 = x_2 = x_5, \quad z = 0, 1 \tag{11}$$

(C)

$$x_1 = x_2 = x_5, \quad z = 0$$

and

$$x_1 = x_3 = x_5, \quad z = 1 \tag{12}$$

Equations (7)-(9) subject to the boundary conditions (10),(11) or (12) constitute the characteristic value problem to the determination of R (and hence of R_c), using our recent direct method for solving several characteristic value problems, described below.

Let $\mathbf{m}$, $\mathbf{n}$ and $\bar{\mathbf{n}}$ be three integer sets

$$\mathbf{m} = \{m_1, \cdots, m_n\}, \ 1 \leq m_1 < m_2 < \cdots < m_n \leq 2n,$$

$$\mathbf{n} = \{n_1, \cdots, n_n\}, \ 1 \leq n_1 < n_2 < \cdots < n_n \leq 2n,$$

$$\bar{\mathbf{n}} = \{1, 2, \cdots, 2n\} - \mathbf{n}, \ 1 \leq \bar{n}_1 < \bar{n}_2 < \cdots \bar{n}_n \leq 2n$$

and let $M[\mathbf{m}, \bar{\mathbf{n}}]$ be the matrix obtained by taking the elements of M with row subscripts from $\mathbf{m}$ and column subscripts from $\bar{\mathbf{n}}$.

Consider the $2n \times 2n$ mixed boundary value problem on the z interval $(0, 1)$:

$$\frac{d\mathbf{x}}{dz} = A(\vec{\rho})\mathbf{x}, \tag{13}$$

$$x_i(0) = 0 \quad \text{for} \quad i \in \mathbf{n} \tag{14}$$

$$x_i(1) = 0 \quad \text{for} \quad i \in \mathbf{m} \tag{15}$$

where $\mathbf{x} = [x_1, x_2, \cdots, x_{2n}]^T$, $A(\vec{\rho}) = A(\rho_1, \cdots, \rho_k)$ is a $2n \times 2n$ matrix with k ρ's as its parameters. The problem is to determine the values of ρ_i's such that the above system is solvable. We have obtained the following theorem which forms the basis of our method for solving the several characteristic value problems arising in the linear theory of thermal convection.

Theorem 1 *The necessary and sufficient condition for the existence of non-trivial solutions of* (13)-(15) *is*

$$det(E(\vec{\rho})) = 0, \ \ where \ \ E(\vec{\rho}) = exp(A(\vec{\rho}))[\mathbf{m}, \bar{\mathbf{n}}]. \tag{16}$$

Furthermore, the number of linearly independent solutions equals the dimension of the null space of E.

The above theorem shows that the characteristic values are simply the solutions of the algebraic equation (16), easily obtainable using some standard numerical method such as the Newton-Raphson method. In thermal convection problems, however we are interested in finding the *critical* or minimum ones among these values, e.g. the critical Rayleigh number R_c. Generally, if we want to find the minimum characteristic value for, say, the *first* parameter ρ_1, our problem can be formulated as a constrained optimisation problem:

Minimize ρ_1, **subject to** $det(E(\vec{\rho})) = 0$.

Many subroutines are available for solving this constrained nonlinear programming problem. One may first convert this constrained problem to an unconstrained one by introducing a penalty term in the objective function, then apply unconstrained optimisation subroutines. Our numerical experiments show that this optimisation approach is not a very good way to find the critical values, while the following alternative approach has proved successful.

As we know the equation

$$f(\vec{\rho}) \equiv det(E(\vec{\rho})) = 0$$

generally defines a function

$$\rho_1 = \rho_1(\rho_2, \cdots, \rho_k)$$

in some open set of R^{k-1}. At the critical value ρ_1^*,

$$\frac{\partial \rho_1}{\partial \rho_i} = 0, \quad i = 2, \cdots, k.$$

Implicit differentiation gives

$$\frac{\partial f}{\partial \rho_i} = 0, \quad i = 2, \cdots, k.$$

Thus the critical value of ρ_1 can be found by solving the system of k equations

$$f = 0 \tag{17}$$

$$\frac{\partial f}{\partial \rho_i} = 0, \quad i = 2, \cdots, k. \tag{18}$$

We summarise this result in Theorem 2.

Theorem 2 *The necessary condition of ρ_1^* being a critical value is that there are $\rho_i^*,\ \ i = 2, \cdots, k$ such that $\vec{\rho}^* = (\rho_1^*, \cdots, \rho_k^*)$ satisfies the equations* (17)-(18).

In most cases these partial derivatives are not given explicitly, so we replace them by difference quotients with appropriately small $\triangle \rho_i$, $i = 2, \cdots, k$.

Returning now to our characteristic value problem (7)-(12), the corresponding sets **m** and n in Theorem 1 for the above boundary types are

$$(A)\, \mathbf{m} = \mathbf{n} = \{1, 3, 5\};\ \ (B)\, \mathbf{m} = \mathbf{n} = \{1, 2, 5\};\ \text{ and }\ (C)\, \mathbf{m} = \{1, 3, 5\},\ \ \mathbf{n} = \{1, 2, 5\}$$

respectively.

Let $f(a, R) = det(E(a, R))$ and $g(a, R) = (f(a+\Delta a, R) - f(a - \Delta a, R))/2\Delta a$, $\Delta a = 10^{-10}$. Solving the system (17), (18) $f = g = 0$ for a and R, we readily obtain with absolute case using *Mathematica* the following results for the three boundary types, which coincide with the results of Chandrasekhar (see pp.43 [2]).

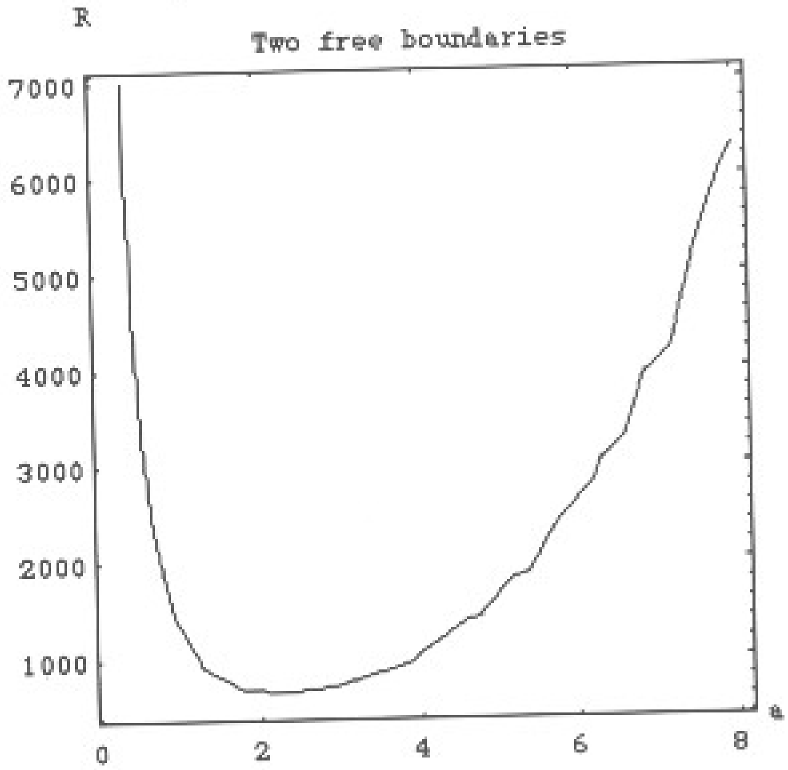
Boundary Type	a_c	R_c	f	g
(A)	2.22144	657.511	4.58212E-6	1.16611E-6
(B)	3.11632	1707.76	1.07249E-6	5.63881E-7
(C)	2.68232	1100.65	-1.19572E-6	-4.25531E-6

Using *Mathematica* with **m[a_, R_]** representing the matrix $A(a, R)$, and **fa[a_, R_]**, **fb[a_, R_]**, **fc[a_, R_]** representing $f(a, R) = det(E(a, R))$ for the three boundary types (A), (B) and (C) respectively, the contour graphs $f(a, R) = 0$ were readily obtained. *Notice the ease of change of boundary conditions, by merely changing some numbers in* **f[a_, R_]** !!!

From these contour graphs we can easily obtain the initial approximations for the critical values a_c and R_c. The corresponding accurate values were then found by solving the equations $f = g = 0$ using the *Mathematica* subroutine **FindRoot** with **g [a_, R_]** representing g.

```
In[1]:=
m[a_,R_]:={{0,1,0,0,0,0},{0,0,1,0,0,0},{0,0,0,1,0,0},
{-a^4,0,2 a^2,0,R a^2,0},{0,0,0,0,0,1},{-1,0,0,0,a^2,0}}
In[2]:=
fa[a_,R_]:=Det[MatrixExp[m[a,R]][[{1,3,5},{2,4,6}]]]
```

```
ContourPlot[fa[a,R],{a,0.1,8},{R,500,7000},Contours→ {0},
ContourShading → False, PlotLabel → "Two free boundaries",
AxesOrigin → Automatic, Axes → {True, True}, AxesLabel → {a, R}]
```



Out[3]=

-ContourGraphics-

In[4]:=

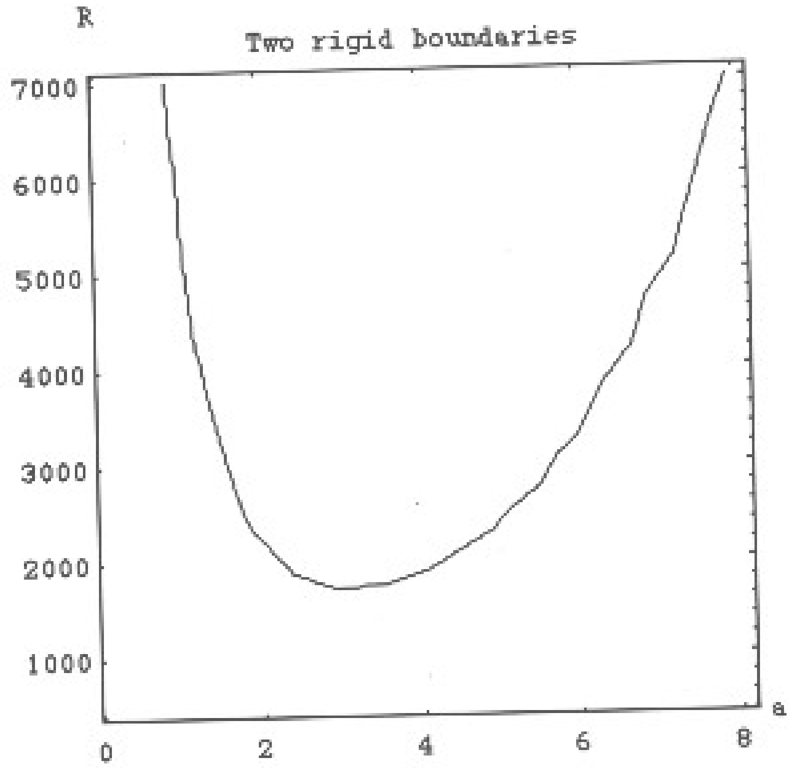
```
ga[a_,R_]:=0.5 10^(10)(fa[a+10^(-10),R]-fa[a-10^(-10),R])
FindRoot[{fa[a,R]==0,ga[a,R]==0},{a,2.0,2.2},{R,500,700}]
```

Out[5]=

{a → 2.22144, *R* → 657.511}

In[6]:=

```
fb[a_,R_]:=Det[MatrixExp[m[a,R]][[{1,2,5},{3,4,6}]]]
ContourPlot[fb[a,R],{a,0.1,8},{R,500,7000},Contours→ {0},
ContourShading,PlotLabel→ "Two rigid boundaries",
AxesOrigin→ Automatic, Axes → {True, True}, AxesLabel → {a, R}]
```



Out[7]=

-ContourGraphics-

In[8]:=

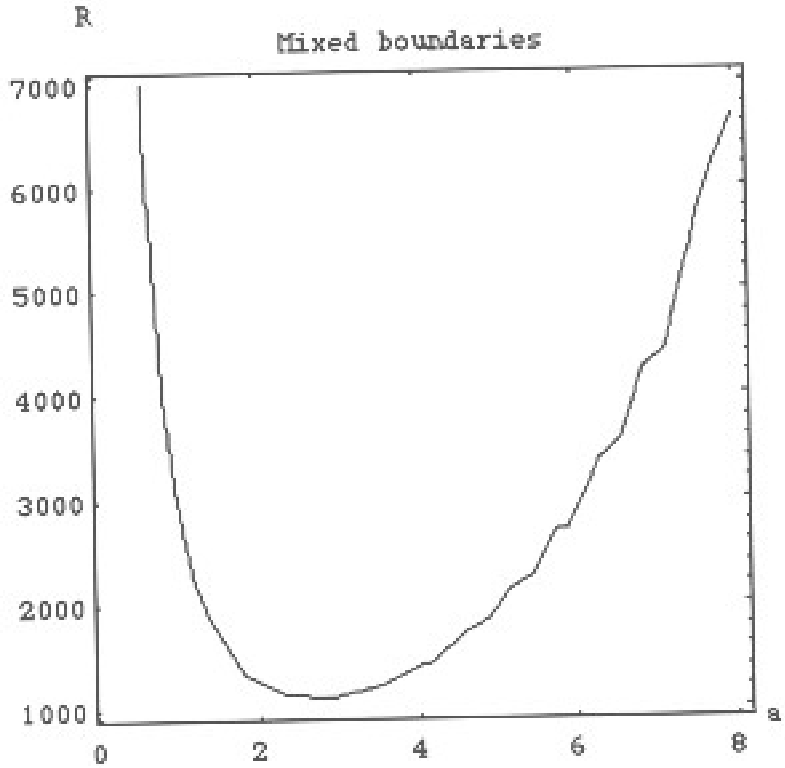
```
gb[a_,R_]:=0.5 10^10 (fb[a+10^(-10),R]-fb[a-10^(-10),R])
FindRoot[{fb[a,R]==0,gb[a,R]==0},{a,3.0,3.2},{R,1500,1600}]
```

Out[9]=

{a → 3.11632, *R* → 1707.76}

In[10]:=

```
fc[a_,R_]:=Det[MatrixExp[m[a,R]][[{1,3,5},{3,4,6}]]]
ContourPlot[fc[a,R],{a,0.1,8},{R,1000,7000},Contours → {0},
ContourShading → False, PlotLabel → "Mixed boundaries",
AxesOrigin→ Automatic, Axes → {True, True}, AxesLabel → {a, R}]
```



Out[11]=

-ContourGraphics-

In[12]:=

```
gc[a_,R_]:=0.5 10^10 (fc[a+10^(-10),R]-fc[a-10^(-10),R])
FindRoot[{fc[a,R]==0,gc[a,R]==0},{a,2.5,2.7},{R,1000,1200}]
```

Out[13]=

$\{a \to 2.68232, R \to 1100.65\}$

2 Thermal instability of a fluid sphere

The thermal instability of an incompressible fluid sphere heated from within by a uniform distribution of heat sources and in equilibrium under its own gravitation has been considered by Chandrasekhar [2], Jeffreys and Bland [3], and Backus [4].

Based on the principle of exchange of stabilities, the linearized equations (derived in [2] and [3] hence not reproduced here) governing the onset of stationary convection in a sphere with a free bounding surface, may be combined into the single sixth order differential equation for the perturbation in the radial velocity $W(r)$

$$D^6W + 6/rD^5W - 6/r^2D^4W + 2c_1W = 0 \tag{19}$$

subjet to the boundary conditions

$$W = D^2W = D^4W + 4/rD^3W = 0, \text{ at } r = a, 1 \tag{20}$$

where $D = d/dr$, $a << 1$ and c_1 may be regarded as "Rayleigh" number.

A solution of Equation (19) which satisfies the boundary conditions (20) and is not zero everywhere is possible only when c_1 takes on a sequence of determinate characteristic values. In the present connection we are interested only in the lowest of these characteristic values, the critical "Rayleigh" number at which convection will begin in an initially cool sphere which begins to warm up internally, or the "Rayleigh" number at which convection will cease in a sphere of fluid losing heat through its surface.

The above eigenvalue problem for the determination of the lowest eigenvalue c_1 has been considered in [2, 3, 4] using a variety of excessively lengthy and extremely laborious techniques. Jeffreys and Bland [3] computed the lowest eigenvalue by an ineffective variational procedure as well as an "exact" procedure applicable only for the special case of a free bounding surface.

Chandrasekhar [2] used a more incisive variational technique to obtain quite accurate estimates of the lowest eigenvalues.

Variational estimates of the eigenvalues however suffer from the disadvantage that they are upper bounds, which in principle cannot bracket the true values. This has prompted Backus [4] to compute the eigenvalues by a very laborious technique which brackets and exhibits the eigenvalues as the zeros of a certain explicit meromorphic function of a single complex variable and, as a by-product, yields expansions for the eigenfunctions in series of spherical Bessel functions.

This has recently motivated us to try and solve the problem by developing a "non-tedious" and user friendly practical approach. Surprisingly, to our best knowledge and belief no one has attempted to solve the problem using the well known finite difference method, even in recent years with the availability of modern computing software.

With this approach, we subdivide the interval $[a, 1]$ in N subintervals of width $h = (1-a)/N$. We denote the point $r_i = a + ih$ and $w_i = W(r_i)$, $i = 0, 1, \cdots, N$. Using the standard central difference approximation of derivatives, Equation (19) and boundary conditions (20) reduce to the linear system

$$A(c_1)\vec{w} = 0 \tag{21}$$

where $A(c_1)$ is an $(N-1) \times (N-1)$ square matrix with a parameter c_1 and $\vec{w} = (w_1, w_2, \cdots, w_{N-1})^T$. The requirement for the existence of non zero solutions $\vec{w}$ is

$$det(A(c_1) = 0. \tag{22}$$

Further, it is easy to see that the matrix $A(c_1)$ has the form

$$A(c_1) = M + 2c_1 I_{N-1} \tag{23}$$

where M is a sparse constant matrix and I_{N-1} is the identity matrix of order $N-1$. Therefore Equation (22) can be equivalently stated as

c_1 is an eigenvalue of the matrix $-0.5M$.

For our problem we seek the lowest eigenvalue of this matrix. The algorithm is hence very simple. It only consists of two steps:

Step1 From Equation (19) to form the matrix M using finite difference approximations for derivatives.

Step2 Find the smallest eigenvalue of the matrix $-0.5M$.

The following code of *Mathematica* is the implementation of the above algorithm.

```
In[1]:=
a=0.00001;
Nm=450;
h=(1 - a)/(Nm+1);
r[k_]=a + k*h;
m=Table[If[i==j, -20/h^6 -36/(r[i]^2*h^4),
If[j==i+1,15/h^6 +15/(r[i]*h^5) + 24/(r[i]^2*h^4),
If[j==i+2,-6/h^6 - 12/(r[i]*h^5) - 6/(r[i]^2*h^4),
If[j==i+3,1/h^6 + 3/(r[i]*h^5),
If[j==i-1 && i¿1,15/h^6 - 15/(r[i]*h^5) + 24/(r[i]^2*h^4),
If[j==i-2 && i¿2,-6/h^6 + 12/(r[i]*h^5) - 6/(r[i]^2*h^4),
If[j==i-3 && i¿3,1/h^6 - 3/(r[i]*h^5),0],0],0],0],0],0],0],
```

```
i,Nm,j,Nm];
m[[1,1]]=m[[1,1]]+6/h^6 - 12/(r[1]*h^5) + 6/(r[1]^2*h^4)
+8*h /(a*(1-2*h/a)) (1/h^6 - 3/(r[1]*h^5));
m[[1,2]]=m[[1,2]]-(1/h^6 - 3/(r[1]*h^5)) (1+2*h/a)/(1-2*h/a);
m[[2,1]]=m[[2,1]]-(1/h^6 - 3/(r[2]*h^5));
m[[Nm,Nm]]=m[[Nm,Nm]]+6/h^6 + 12/(r[Nm]*h^5) + 6/(r[Nm]^2*h^4)
-8*h /(1+2*h) (1/h^6 + 3/(r[Nm]*h^5));
m[[Nm,Nm-1]]=m[[Nm,Nm-1]]-(1/h^6 + 3/(r[Nm]*h^5)) (1-2*h)/(1+2*h);
m[[Nm-1,Nm]]=m[[Nm-1,Nm]]-(1/h^6 + 3/(r[Nm-1]*h^5));
Eigenvalues[-0.5*m][[Nm]]
Out[1]=
3091.68
```

In the above code $Nm = N - 1$ represents the dimension of the matrix M,where the number of subintervals N is chosen to guarantee the required accuracy.

A comparison of the critical "Rayleigh" number c_1 obtained by our algorithm with the currently available results obtained by very laborious "exact" or "approximate" variational techniques is shown below for the case of a free bounding surface.

Value obtained by our algorithm	Jeffreys & Bland 's "exact" value	Backus' "exact" value	Chandrasekhar's variational value	Jeffreys & Bland 's variational value
3091.68	3091±2	3091.2	3091.2	3202

This table shows the ineffectiveness of the variational procedure used by Jeffreys and Bland [3] and the superiority of Chandrasekhar's [2] more incisive variational procedure. What is not apparent from the table is the excessive length and labour involved in these techniques.

Our simple two step algorithm readily gives with literally only a few lines of code an accurate value for the critical "Rayleigh" number.

Finally, we would like to draw attention to the fact that, since we only calculate the smallest eigenvalue of the sparse matrix $-0.5M$, the total amount of calculation is reduced if the inverse power method [5] is employed.

3 Conclusions

Two illustrations of our recent progress in the theory of thermal instability facilitated by the use of *Mathematica* have been presented.

Firstly, the classical Bénard problem has been investigated using our recently developed direct method. This allows a simple, versatile, accurate, rigorous, unified and trasparent treatment of the several characteristic value problems arising in the Bénard and previously unsolved related problems arising in the linear theory of thermal instability in both Newtonian and viscoelastic fluids.

Secondly, the finite difference method with a few modifications has been successfully applied to obtain a simple and elegant two step algorithm for the determination of the critical "Rayleigh" number for the onset of convection in a fluid sphere heated within. With the aid of *Mathematica*, this algorithm gives accurate results with absolute ease. A test comparison with the best currently available results obtained by laborious techniques for the case of a fluid sphere with a free bounding surface clearly reveals the accuracy, superiority and practicality of our algorithm. The method can be readily applied to the case of a rigid bounding surface, and also to the treatment of convection in spherical shells.

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