

PFC/RR-90-7

**Variational Solutions of the
Transport Equation**

E.A. Chaniotakis
J.P. Freidberg

November 1990

Plasma Fusion Center
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139 USA

This work was supported by the Princeton Plasma Physics Lab under sub-
contract No.: S-02969-A.

Variational Solutions of the Transport Equation

E.A. Chaniotakis, J.P. Freidberg

Massachusetts Institute of Technology

Abstract

In this paper, the extremal principle which results in variational solutions to the general transport equation is presented. Due to the non-self adjoint character of the transport equation the variational solutions are obtained by applying the variation to the fluctuation alone. The effectiveness of the method is demonstrated for various forms of the phenomenological coefficients. In general the accuracy of the method is very good (errors < 1%). The execution time is reduced by an order of magnitude when compared to standard finite differencing techniques. The procedure is extended to a set of N differential equations.

1 Introduction

The importance of variational methods in the development of theoretical physics, both classical and quantum (modern), has long been appreciated. Extremal principles have given rise to the energy concept which forms the basis for visualizing the behavior of complex mechanical systems. [1] For example the equations of motion, and thus the behavior, of the system shown in Fig. 1 can not be easily deduced from simple force displacement considerations. However, by considering the energy (both kinetic and potential) associated with the system the equations of motion can be deduced in a

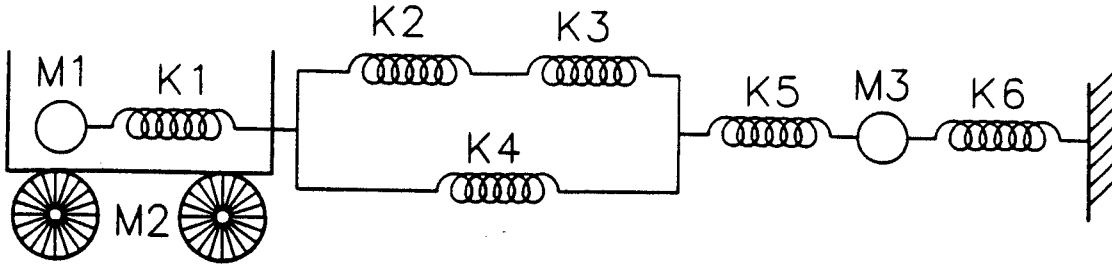


Figure 1: A typical mechanical system whose equations of motion are difficult to obtain by simply considering force balance relations. The equations can be obtained easily by considering the Lagrangian of the system

straight forward manner by considering the extremal of a function “the Lagrangian” which is related to macroscopic energy content of the system.[2]

In addition to this conceptual advantage, extremal “variational” principles can be effective in the construction of solutions to mechanical problems. In this case, the equations describing the behavior of the system are known apriori and their solution, under certain constraints (boundary conditions, and initial conditions), is obtained through the use of variational principles.[3]

Since transport equations in general characterize dissipative systems, the Lagrangian formulation of such a problem falls outside the “classical” range of variational applications.[2,4] In general the Lagrangian formulation of a dissipative system may be considered an extension of classical variational calculus to non-self-adjoint problems. This extension is made possible by applying the variational principle to the fluctuation alone.

In this work the variational formulation of the transport equation is presented in its generality. First, a brief review of the variational procedure,

by which solutions to a certain set of equations can be obtained, is presented in section 2. Second, in section 3 the theory behind the variational formulation for dissipative (non-self-adjoint) systems is developed. Third, the variational formulation of the heat equation including both non-linear thermal conductivity and convective terms is presented in section 4, and solutions obtained by the variational methods are compared to “exact” solutions in section 6. Finally, in section 7 the variational formulation for a system of N transport equations is presented.

2 Variational formulation: General Remarks

The equations describing the behavior of a physical system are put in the variational form by introducing the integral

$$\mathcal{L} = \int L dx \quad (1)$$

where L , the Lagrangian density, is a *function of functions* [5] of the basic system parameters (i.e. space and time), and the generalized coordinates (i.e. dependent variables) $\alpha_1, \dots, \alpha_n$.

$$L = L(\alpha_j; f(x, t)) \quad (j = 1, \dots, n) \quad (2)$$

where $f(x, t)$ is the function characterising the system.

In general, the solution of physical problems via the variational formulation is a three step process. First, the functional \mathcal{L} “Lagrangian” must be found whose first variation, $\delta\mathcal{L}$, yields the equation(s) describing the system as its “Euler equation”. Second, a set of functions characterizing the solution must be determined. These “trial functions”, which are given in terms of certain number of undetermined coefficients, the generalized coordinates, $\alpha_1, \dots, \alpha_n$, are in turn substituted into the functional \mathcal{L} . Third, by taking the variations

$$\frac{\delta\mathcal{L}}{\delta\alpha_j} = 0 \quad (j = 1, \dots, n) \quad (3)$$

a set of equations (differential or algebraic) are derived whose solution gives the values of α_j required for making the Lagrangian stationary.[1,3] Once the third step has been completed the solution is found by substituting the values of α_j into the assumed trial functions.

In section 4, the variational formulation of the heat equation will be obtained by following the above three steps.

3 Lagrangian Formulation of Dissipative Systems

It is known from studies of classical thermodynamics that entropy production gives a measure of the approach to equilibrium of physical systems exhibiting reversible processes.[6] It is then important to investigate whether there is any function which for the case of dissipative systems could correspond to the role that the Lagrangian function plays in the development of classical and quantum mechanics.

It has been shown that for dissipative systems there exists the quantity

$$d\Phi = \int_V \sum_j F_j dQ_j dV \leq 0 \quad (4)$$

which holds during the time evolution of the system without reference to the relation between the forces F_j and the fluxes Q_j . [7,8] The inequality given by Eq. (4) is so general that it has been called a universal evolution criterion valid throughout the whole range of macroscopic physics.[9] In general the function Φ is called the “local potential”. This local potential if it exists for the physical system under investigation is equivalent to the Lagrangian used in classical mechanics. By investigating the simple heat equation it is shown that there is a function corresponding to the heat equation which corresponds to Eq. (4).

The simple heat conduction equation of fixed density normalized to one is given by

$$c_v \frac{\partial T}{\partial t} = -\frac{\partial q_j}{\partial x_j} \quad (5)$$

with q_j representing the heat flux, and where c_v is the specific heat.

By considering the domain of solutions of Eq. (5) within a volume V with a boundary surface S , the families of temperature distributions of the form

$$T = \hat{T}(x_j, t) + \delta T(x_j, t) \quad (6)$$

where \hat{T} is the appropriate macroscopic temperature distribution and where δT are small variations around the macroscopic distribution represent the solution of Eq. (5). For the Fourier law

$$q_j = -\kappa(T) \frac{\partial T}{\partial x_j} \quad (7)$$

the thermal conductivity κ may be written as

$$\kappa(T) = \kappa(\hat{T} + \delta T) = \hat{\kappa} + \delta\kappa \quad (8)$$

and similarly the specific heat may be written as

$$c_v = \hat{c}_v + \delta c_v \quad (9)$$

By multiplying Eq. (5) by $-\delta T$ and by substituting Eq. (7) it follows that

$$-c_v \left(\frac{\partial \hat{T}}{\partial t} + \frac{\partial(\delta T)}{\partial t} \right) \delta T = -\frac{\partial}{\partial x_j} \left(\kappa \frac{\partial T}{\partial x_j} \right) \delta T \quad (10)$$

which reduces to

$$-c_v \frac{\partial \delta T}{\partial t} \delta T = c_v \frac{\partial \hat{T}}{\partial t} \delta T - \frac{\partial}{\partial x_j} \left(\kappa \frac{\partial T}{\partial x_j} \delta T \right) + \kappa \frac{\partial T}{\partial x_j} \frac{\partial \delta T}{\partial x_j} \quad (11)$$

and which is equivalent to

$$-\frac{1}{2} \frac{\partial (\delta T)^2}{\partial t} = \frac{\partial \hat{T}}{\partial t} \delta T - \frac{1}{c_v} \frac{\partial}{\partial x_j} \left(\kappa \frac{\partial T}{\partial x_j} \delta T \right) + \frac{\kappa}{c_v} \frac{\partial T}{\partial x_j} \frac{\partial \delta T}{\partial x_j} \quad (12)$$

Integrating Eq. (12) over the volume V results in

$$\begin{aligned} -\frac{1}{2} \frac{\partial}{\partial t} \int_V (\delta T)^2 dV &= \int_V \left[\frac{\partial \hat{T}}{\partial t} \delta T + \frac{\kappa}{2c_v} \delta \left(\frac{\partial T}{\partial x_j} \right)^2 + \kappa \frac{\partial T}{\partial x_j} \delta T \frac{\partial}{\partial x_j} \left(\frac{1}{c_v} \right) \right] dV \\ &\quad - \int_S \frac{\kappa}{c_v} \frac{\partial T}{\partial x_j} \delta T dS \end{aligned} \quad (13)$$

and by Integrating Eq. (13) over time the following results

$$\begin{aligned} -\frac{1}{2} \int_V (\delta T)^2 dV &= \int_t \int_V \left[\frac{\partial \hat{T}}{\partial t} \delta T + \frac{\kappa}{2c_v} \delta \left(\frac{\partial T}{\partial x_j} \right)^2 + \kappa \frac{\partial T}{\partial x_j} \delta T \frac{\partial}{\partial x_j} \left(\frac{1}{c_v} \right) \right] dV dt \\ &\quad - \int_t \int_S \frac{\kappa}{c_v} \frac{\partial T}{\partial x_j} \delta T dS dt \end{aligned} \quad (14)$$

Since the left hand side term of the above equation is negative definite, the right hand side is always less than or equal to zero. Assuming that $\delta T \ll \hat{T}$ and substituting Eq. (8) into the right hand side of Eq. (14) gives to the first order

$$\int_t \int_V \left[\frac{\partial \hat{T}}{\partial t} \delta T + \hat{\kappa} \frac{\partial}{\partial x_j} \left(\frac{1}{\hat{c}_v} \delta T \right) \frac{\partial T}{\partial x_j} \right] dV dt - \int_t \int_S \frac{\hat{\kappa}}{\hat{c}_v} \frac{\partial T}{\partial x_j} \delta T dS dt \leq 0 \quad (15)$$

If the temperature is specified on the boundary S (i.e. if $\delta T = 0$ on the boundary) or if the fluxes across the boundary are zero the surface integral in Eq. (15) vanishes. Therefore the variation

$$\int_t \int_V \left[\frac{\partial \hat{T}}{\partial t} \delta T + \hat{\kappa} \frac{\partial}{\partial x_j} \left(\frac{\delta T}{c_v} \right) \frac{\partial T}{\partial x_j} \right] dV dt \leq 0 \quad (16)$$

is always less than zero, and it is equal to zero when the temperature distribution corresponding to \hat{T} is reached.

Similar arguments can be developed even if the time integration of Eq. (13) is not performed. In that case the quantity

$$\int_V \left[\frac{\partial \hat{T}}{\partial t} \delta T + \hat{\kappa} \frac{\partial}{\partial x_j} \left(\frac{\delta T}{c_v} \right) \frac{\partial T}{\partial x_j} \right] dV \quad (17)$$

can be positive or negative but it becomes zero when the temperature corresponding to the macroscopic distribution \hat{T} is reached. Therefore, the achievement of the macroscopic distribution \hat{T} can be characterized by the extremum condition

$$\left. \frac{\delta \mathcal{L}(\hat{T}, T)}{\delta T} \right|_{\hat{T}} = 0 \quad (18)$$

with the subsidiary condition

$$T = \hat{T} \quad (19)$$

The functional \mathcal{L} is given by

$$\mathcal{L} = \int_V \left[T \left(\frac{\partial \hat{T}}{\partial t} \right) + \frac{1}{2} \frac{\hat{\kappa}}{c_v} \left(\frac{\partial T}{\partial x_j} \right)^2 \right] dV \quad (20)$$

where for simplicity it has been assumed that the specific heat c_v is independent of temperature, T .

The functional \mathcal{L} will henceforth be called the Lagrangian of the system. The optimization operation indicated by Eq. (18) shows that the functional \mathcal{L} has as its Euler-Lagrange equation the original heat transport equation (5). A detailed proof of this point is given in the next section for a specific example.

4 Variational formulation of the heat equation

In order to gain insight into the workings of the variational formulation, and appreciation of its power in finding solutions to the diffusion problem, various simple examples are presented.

The heat transport equation, in cylindrical geometry of unit radius and of normalized constant density, is given by

$$\frac{\partial T(\rho, t)}{\partial t} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \left[\kappa(T, \rho, t) \frac{\partial T(\rho, t)}{\partial \rho} - v(T, \rho, t) T(\rho, t) \right] + S(T, \rho, t) \quad (21)$$

$$\frac{\partial T(0, t)}{\partial \rho} = 0 \quad (22)$$

$$T(1, t) = 0 \quad (23)$$

$$T(\rho, 0) = f(\rho) \quad (24)$$

Note that Eq. (21) is, in general, non-linear since the thermal conductivity, κ , the convective velocity, v , and the source term, S have been written as functions of temperature, T , space, ρ , and time t .

For the above problem the Lagrangian \mathcal{L} is given by

$$\mathcal{L} = \int_A L dA \quad (25)$$

where the integration is over the cross sectional area of the cylinder, and the Lagrangian density L is defined by

$$L = T \frac{\partial \hat{T}}{\partial t} + \frac{1}{2} \hat{\kappa} \left(\frac{\partial T}{\partial \rho} \right)^2 - \hat{v} \hat{T} \frac{\partial T}{\partial \rho} - I \quad (26)$$

where the quantity I in the last term of Eq. (26) is given by

$$I \equiv \int_{\hat{T}}^T S dT \quad (27)$$

where \widehat{T} is the macroscopic temperature. Therefore, the Lagrangian \mathcal{L} becomes

$$\mathcal{L} = \int_0^1 \int_0^{2\pi} \rho d\rho d\theta \left[T \frac{\partial \widehat{T}}{\partial t} + \frac{1}{2} \widehat{\kappa} \left(\frac{\partial T}{\partial \rho} \right)^2 - \widehat{v} \widehat{T} \frac{\partial T}{\partial \rho} - I \right] \quad (28)$$

In the above equation it is assumed, following the formulation presented in section 3, that the temperature distribution T is made up of the appropriate macroscopic temperature distribution \widehat{T} , plus small variations of the temperature, δT , about the distribution \widehat{T} [4]

$$T = \widehat{T}(\rho, t) + \delta T(\rho, t) \quad (29)$$

The thermal conductivity, κ , and the convective velocity, v , in Eq. (28), are arbitrary functions of temperature and are evaluated at the macroscopic temperature \widehat{T} so they are appropriately labeled $\widehat{\kappa}$, and \widehat{v} .

The Lagrangian \mathcal{L} is thus a function of both the total temperature T and the macroscopic temperature \widehat{T} . The crucial feature to note is that in taking the variations of \mathcal{L} the quantities accented with a ($\widehat{\quad}$) are not subject to variation. The first variation of Eq. (28) gives

$$\delta \mathcal{L} = 2\pi \int_0^1 \left[\delta T \frac{\partial \widehat{T}}{\partial t} + \widehat{\kappa} \frac{\partial T}{\partial \rho} \frac{\partial (\delta T)}{\partial \rho} - \widehat{v} \widehat{T} \frac{\partial (\delta T)}{\partial \rho} - S \delta T \right] \rho d\rho \quad (30)$$

where by assuming poloidal symmetry the integration over the poloidal angle has been performed. Since the relation between δT and $\partial(\delta T)/\partial \rho$ is not known, a simple integration by parts of the second and third terms in the right hand side of Eq. (30) yields

$$\begin{aligned} \delta \mathcal{L} = \int_0^1 \left[\frac{\partial \widehat{T}}{\partial t} - \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \widehat{\kappa} \frac{\partial T}{\partial \rho} \right) + \frac{1}{\rho} \frac{\partial}{\partial \rho} (\rho \widehat{v} \widehat{T}) - S \right] \delta T \rho d\rho \quad (31) \\ + \rho \widehat{\kappa} \frac{\partial T}{\partial \rho} \delta T \Big|_0^1 - \rho \widehat{v} \widehat{T} \delta T \Big|_0^1 \end{aligned}$$

Where the factor of 2π , being a constant, has been neglected from the above equation.

From Eq. (23) it is seen that the value of the temperature, T , at the boundary of the cylinder ($\rho = 1$) has been specified (i.e. $\delta T(1, t) = 0$). Therefore the last two terms in Eq. (31) are equal to zero. Now that the variation has been calculated, set $T = \hat{T}$, $\hat{v} = v$, $\kappa = \hat{\kappa}$, and Eq. (31) becomes

$$\delta\mathcal{L} = \int_0^1 \left[\frac{\partial T}{\partial t} - \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \kappa \frac{\partial T}{\partial \rho} \right) + \frac{1}{\rho} \frac{\partial}{\partial \rho} (\rho v T) - S \right] \delta T \rho d\rho \quad (32)$$

Thus, in order for \mathcal{L} to be stationary (i.e. $\delta\mathcal{L} = 0$) for arbitrary variations, δT , it is necessary that the quantity within the square brackets in Eq. (32) must vanish. Therefore, the *necessary* and *sufficient* condition [1] for the vanishing of $\delta\mathcal{L}$ under arbitrary δT variations is that T satisfies the original equation (21). Therefore, the function T which makes the Lagrangian stationary (i.e. $\delta\mathcal{L} = 0$) is also a solution to the original equation. It has thus been shown that the ‘‘Euler equation’’ of the Lagrangian given by Eq. (28) is the equation characterizing the system under investigation.

The next step in the variational formulation requires the introduction of the trial function. Such a trial function must be capable of representing, or approximating, the solution of the differential equation. For the heat transport problem under investigation (Eqs. (21, - 24)) a function which models a wide variety of profiles is

$$T = T_0(1 - \rho^2) \exp [\alpha_1 \rho^2 + \alpha_2 \rho^4] \quad (33)$$

The coefficients, $T_0(t)$, $\alpha_1(t)$, and $\alpha_2(t)$, characterize the solution, and they are to be determined as a function of time. Fig. 2 demonstrates the flexibility provided by Eq. (33) in modeling profile shapes. Note that steep, flat,

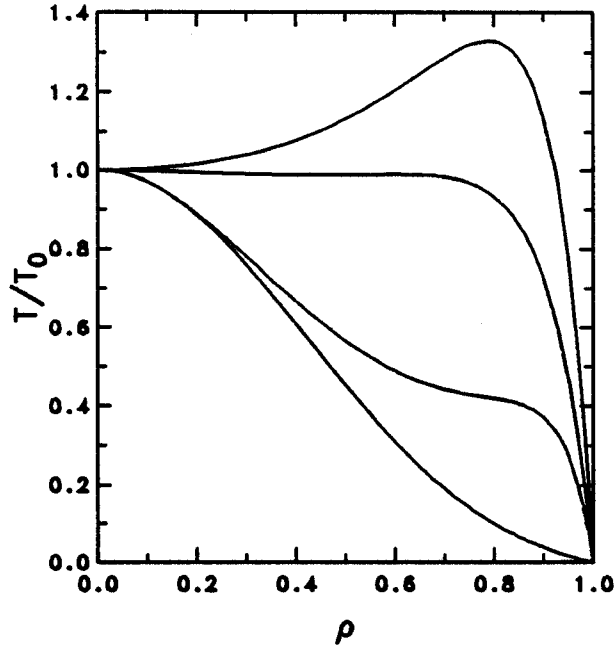


Figure 2: Profile shapes obtained for various values of the parameters α_1 , and α_2 . Note that profile shapes ranging from peaked to flat to hollow can be produced with the trial function Eq. (33).

and hollow profiles can be modeled by appropriately choosing the parameters α_1 , and α_2 .

In accordance with the variational principle the function \hat{T} in Eq. (28) is written as

$$\hat{T} = \hat{T}_0(1 - \rho^2) \exp [\hat{\alpha}_1 \rho^2 + \hat{\alpha}_2 \rho^4] \quad (34)$$

When computing the Euler-Langrange equations the parameters T_0 , α_1 , and α_2 are varied while \hat{T}_0 , $\hat{\alpha}_1$, and $\hat{\alpha}_2$ are held fixed. After the variation one sets $\hat{T}_0 = T_0$, $\hat{\alpha}_1 = \alpha_1$, and $\hat{\alpha}_2 = \alpha_2$. Specifically by substituting the trial function Eqs. (33, 34) into Eq. (28) the extremum of \mathcal{L} in the $(T_0, \alpha_1, \alpha_2)$ space is found by taking the derivatives

$$\left. \frac{\partial \mathcal{L}(T, \hat{T})}{\partial T_0} \right|_{\hat{T}} = 0 \quad (35)$$

$$\left. \frac{\partial \mathcal{L}(T, \hat{T})}{\partial \alpha_1} \right|_{\hat{T}} = 0 \quad (36)$$

$$\left. \frac{\partial \mathcal{L}(T, \hat{T})}{\partial \alpha_2} \right|_{\hat{T}} = 0 \quad (37)$$

subject to the subsidiary conditions

$$\hat{T}_0 = T_0 \quad (38)$$

$$\hat{\alpha}_1 = \alpha_1 \quad (39)$$

$$\hat{\alpha}_2 = \alpha_2 \quad (40)$$

Equations (35 – 37) take the form

$$\begin{aligned} \int_0^1 \left[\frac{\partial T}{\partial T_0} \frac{\partial T}{\partial t} + \kappa \frac{\partial T}{\partial \rho} \frac{\partial}{\partial \rho} \left(\frac{\partial T}{\partial T_0} \right) - v T \frac{\partial}{\partial \rho} \left(\frac{\partial T}{\partial T_0} \right) \right] \rho d\rho \\ - \int_0^1 \left[S \left(\frac{\partial T}{\partial T_0} \right) \right] \rho d\rho = 0 \end{aligned} \quad (41)$$

$$\begin{aligned} \int_0^1 \left[\frac{\partial T}{\partial \alpha_1} \frac{\partial T}{\partial t} + \kappa \frac{\partial T}{\partial \rho} \frac{\partial}{\partial \rho} \left(\frac{\partial T}{\partial \alpha_1} \right) - v T \frac{\partial}{\partial \rho} \left(\frac{\partial T}{\partial \alpha_1} \right) \right] \rho d\rho \\ - \int_0^1 \left[S \left(\frac{\partial T}{\partial \alpha_1} \right) \right] \rho d\rho = 0 \end{aligned} \quad (42)$$

$$\begin{aligned} \int_0^1 \left[\frac{\partial T}{\partial \alpha_2} \frac{\partial T}{\partial t} + \kappa \frac{\partial T}{\partial \rho} \frac{\partial}{\partial \rho} \left(\frac{\partial T}{\partial \alpha_2} \right) - v T \frac{\partial}{\partial \rho} \left(\frac{\partial T}{\partial \alpha_2} \right) \right] \rho d\rho \\ - \int_0^1 \left[S \left(\frac{\partial T}{\partial \alpha_2} \right) \right] \rho d\rho = 0 \end{aligned} \quad (43)$$

Using the chain rule, the time derivative of T becomes

$$\frac{\partial T}{\partial t} = \frac{\partial T}{\partial T_0} \frac{dT_0}{dt} + \frac{\partial T}{\partial \alpha_1} \frac{d\alpha_1}{dt} + \frac{\partial T}{\partial \alpha_2} \frac{d\alpha_2}{dt} \quad (44)$$

where for the trial functions under consideration

$$\frac{\partial T}{\partial T_0} = \frac{T}{T_0} \quad (45)$$

$$\frac{\partial T}{\partial \alpha_1} = T \rho^2 \quad (46)$$

$$\frac{\partial T}{\partial \alpha_2} = T \rho^4 \quad (47)$$

Finally, the equations to be solved can be written in the matrix form

$$\vec{U} = \vec{A}^{-1} \vec{R} \quad (48)$$

Note that we have adapted the convention that the dot-operator ($\dot{}$) denotes differentiation with respect to time. In Eq. (48), \vec{U} is a column vector with components,

$$\vec{U} = \begin{bmatrix} \dot{T}_0 \\ \dot{\alpha}_1 \\ \dot{\alpha}_2 \end{bmatrix} \quad (49)$$

\vec{A} is a 3×3 symmetric matrix,

$$\vec{A} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{12} & A_{22} & A_{23} \\ A_{13} & A_{23} & A_{33} \end{bmatrix} \quad (50)$$

whose elements are given by

$$A_{11} = \frac{1}{T_0^2} \int_0^1 T^2 \rho \, d\rho \quad (51)$$

$$A_{12} = \frac{1}{T_0} \int_0^1 T^2 \rho^3 \, d\rho \quad (52)$$

$$A_{13} = \frac{1}{T_0} \int_0^1 T^2 \rho^5 \, d\rho \quad (53)$$

$$A_{22} = \int_0^1 T^2 \rho^5 d\rho \quad (54)$$

$$A_{23} = \int_0^1 T^2 \rho^7 d\rho \quad (55)$$

$$A_{33} = \int_0^1 T^2 \rho^9 d\rho \quad (56)$$

Note that the elements A_{ij} are independent of the phenomenological coefficients κ , and v , as well as of the source term S . The dependance on κ , v , and S is incorporated into the elements of the column vector \vec{R}

$$\vec{R} = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \end{bmatrix} \quad (57)$$

where for a trial function of the form given by Eq. (33) the elements of \vec{R} are

$$R_1 = \frac{1}{T_0} \int_0^1 \left[-\kappa \left(\frac{\partial T}{\partial \rho} \right)^2 + v T \frac{\partial T}{\partial \rho} + S T \right] \rho d\rho \quad (58)$$

$$R_2 = \int_0^1 \left[-\kappa \frac{\partial T}{\partial \rho} \frac{\partial}{\partial \rho} (\rho^2 T) + v T \frac{\partial}{\partial \rho} (\rho^2 T) + S T \rho^2 \right] \rho d\rho \quad (59)$$

$$R_3 = \int_0^1 \left[-\kappa \frac{\partial T}{\partial \rho} \frac{\partial}{\partial \rho} (\rho^4 T) + v T \frac{\partial}{\partial \rho} (\rho^4 T) + S T \rho^4 \right] \rho d\rho \quad (60)$$

Therefore, Eq. (48) represents a system of coupled non-linear ordinary differential equations in time. The variational formulation has thus converted the original partial differential equation in (ρ, t) to a system of ordinary differential equations in t . Consequently, the system represented by Eq. (48) is less complex, and as we shall see this method is faster than the solution of difference equations required to approximate the partial differential equation.

In the next section we evaluate the validity of the variational formulation, in terms of accuracy, relative to solutions obtained by analytic means, and in terms of accuracy and speed, relative to solutions obtained by finite differencing.

5 Generalized Boundary Conditions

If the solution of Eq. (21) is desired with non zero (constant or time dependent) edge boundary condition i.e. if Eq. (23) has the form

$$T(1, t) = T_1(t) \quad (61)$$

the Lagrangian given by Eq. (28) has to be modified in order to appropriately represent this situation. The alternate variational formulation which takes into account this boundary condition is

$$\begin{aligned} \mathcal{L} = \int_0^1 \rho d\rho \left[T \frac{\partial \hat{T}}{\partial t} + \frac{1}{2} \hat{\kappa} \left(\frac{\partial T}{\partial \rho} \right)^2 - \hat{v} \hat{T} \frac{\partial T}{\partial \rho} - I \right] \\ - \rho \hat{\kappa} \frac{\partial \hat{T}}{\partial \rho} T \Big|_{\rho=1} + \rho \hat{v} \hat{T} T \Big|_{\rho=1} \end{aligned} \quad (62)$$

The Lagrangian given by Eq. (62) contains the “natural boundary condition” of the system,[10] and it has the advantage of allowing trial functions to be substituted that do not satisfy the boundary condition Eq. (61).

The trial function, Eq. (33), can incorporate the non-zero boundary condition Eq. (61) with the following modification

$$T = T_0(1 - \gamma\rho^2) \exp[\alpha_1\rho^2 + \alpha_2\rho^4] \quad (63)$$

where γ is given by

$$\gamma = 1 - \frac{T_1(t)}{T_0 \exp[\alpha_1 + \alpha_2]} \quad (64)$$

The remaining analysis for the formulation of the problem proceeds exactly as the case with zero boundary conditions presented in section 4. The only difference is the addition of the two new boundary terms and the incorporation of the parameter γ in the formulation.

6 Test problems

By assuming various forms for the thermal conductivity κ , the convective velocity v , the source term S , both analytic and/or numerical (finite differencing) solutions of Eqs. (21 – 24) are obtained and the results are compared with solutions obtained via the variational formulation. First, solutions to a single transport equation are investigated under various forms of the phenomenological coefficients κ , and v . Next, the variational procedure is generalized to include several dependent variables and solutions to a coupled set of equations is presented.

The values of the various parameters used in this section are given in arbitrary units since we are interested only in comparing the performance of the variational formulation, and not in extracting specific physical information from the results.

6.1 Linear Problem

By assuming $\kappa = \kappa_0 = \text{const.}$, $v = 0$, and $S = \lambda T$ (where $\lambda = \text{const.}$), the analytic solution of Eqs. (21 – 24) is obtained in terms of the Bessel functions

$$T(\rho, t) = 2 \sum_{j=1}^{\infty} \frac{J_0(\nu_j \rho)}{[J_1(\nu_j)]^2} \exp [(\lambda - \nu_j^2 \kappa_0)t] \int_0^1 \rho f(\rho) J_0(\nu_j \rho) d\rho \quad (65)$$

where J_p is the Bessel function of order p , and where ν_j are the zeros of J_0 i.e. $J_0(\nu_1) = 0$.

In comparing the variational with the analytic results, both the time behavior of the peak temperature, T_0 , and the profile shapes will be considered. For $\kappa = 0.5$, and $\lambda = 1.0$ the time evolution of the peak temperature T_0 , and the profile shapes at time $t = 0.5$ are shown in Fig. 3. Note that both the time evolution of the peak temperature, and the profiles obtained by the analytic and variational methods are in excellent agreement.

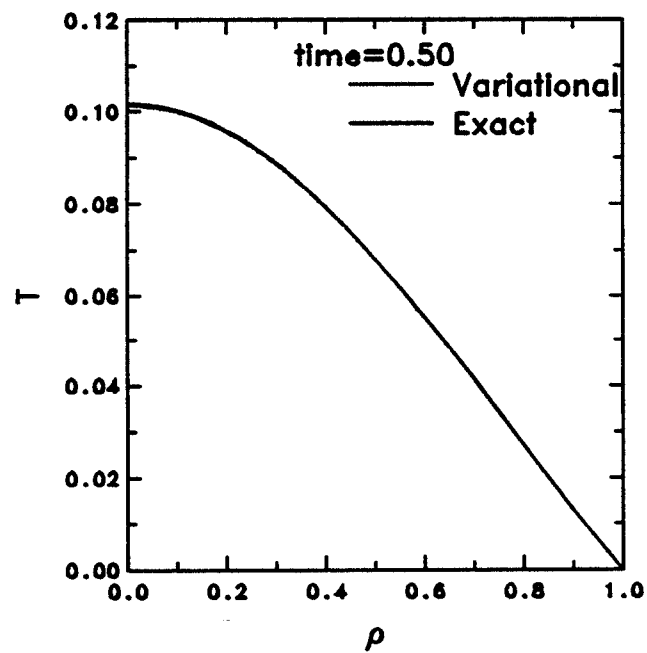
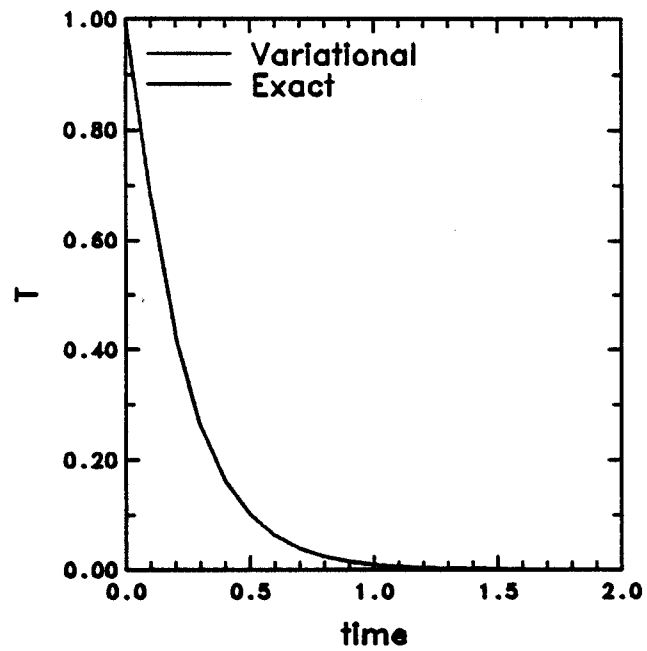


Figure 3: Comparison of the results obtained from the variational and the exact solution of a linear problem. Note that the time evolution of the peak temperature, shown in (a), is in excellent agreement for the two methods. In (b) the profiles are compared at time $t = 0.5$

6.2 Linear problem with convection

Here, the effectiveness of the variational formulation is evaluated for non-zero convection velocity. By taking $\kappa = 0.5 v = v_0 \rho$ (where $v_0 = 0.5$), and $S = 0$ the time evolution of the peak temperature, T_0 , and the profiles at time $t = 0.5$ are shown in Fig. 4. Note that even in the case of convection the solution obtained via the variational formulation is in excellent agreement with the analytic solution.

6.3 Non-Linear problem with heat pulse

By assuming $v = 0$ and by considering a thermal diffusivity of the form

$$\kappa = 0.5 \exp[\rho^2] \quad (66)$$

with a source term given by

$$S = \frac{C_1}{(T + T_1)^{1.5}} + P(\rho, t) \quad (67)$$

the performance of the variational formulation of the transport problem Eq. (21) is investigated. Since the variational formulation is developed for obtaining solutions to the plasma transport equations, the form of the source term S , Eq. (67) has been purposely chosen to model the $1/T^{3/2}$ dependence of the plasma ohmic heating term. T_1 in Eq. (67) is some number different from zero in order to avoid the situation at which the source term S becomes infinite at the plasma edge. The term $P(\rho, t)$ in Eq. (67) is used to simulate a heat pulse of the form.

$$P = \begin{cases} 0 & \text{if } t < t_1 \\ P_0 \exp\left[\frac{(\rho - \rho_0)^2}{\sigma^2}\right] & \text{if } t_1 \leq t \leq t_2 \\ 0 & \text{if } t > t_2 \end{cases} \quad (68)$$

In a physical situation, the term P could represent the heating of a plasma due to externally applied RF or neutral beam heating. For $\rho_0 = 0$, $\sigma = 0.5$,

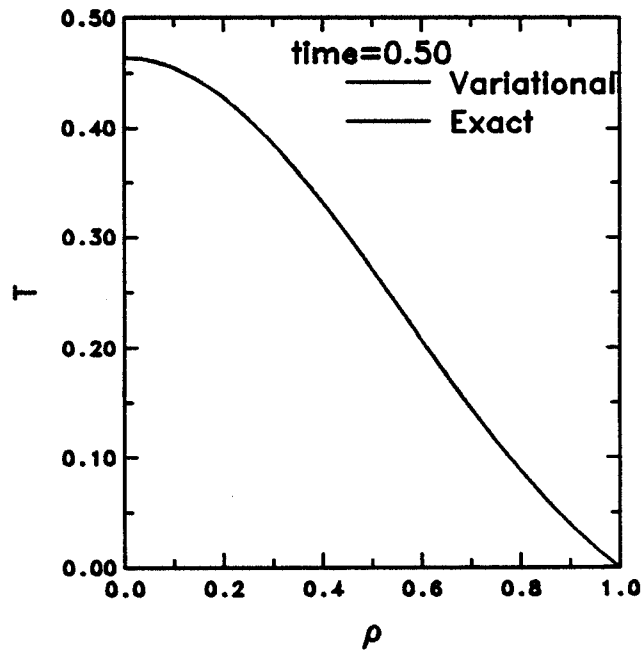
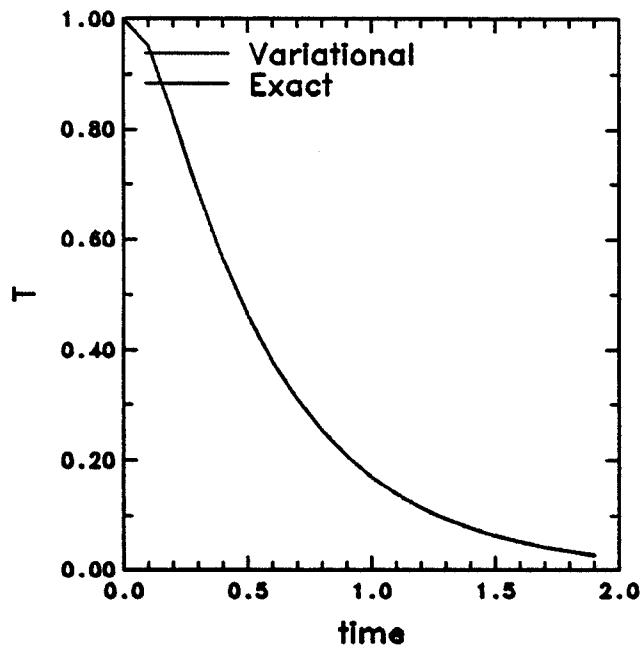


Figure 4: Comparison of the results obtained from the variational and the finite differencing formulation of a linear problem with convection. Note that the time evolution of the peak temperature, shown in (a), is in excellent agreement for the two methods. In (b) the profiles are compared at time $t = 0.5$

Table 1: Comparison of execution times on a VAX computer for the variational and finite differencing methods for the non-linear problem with heat pulse

Method	Time (sec.)
Variational	5.10
Differencing 40 grid points	47.95
Differencing 30 grid points	32.57
Differencing 20 grid points	19.59
Differencing 10 grid points	9.94
Differencing 5 grid points	5.13

$C_1 = 1.0$, $T_1 = 0.5$, and $P_0 = 2.0$ the results for both the variational and the finite differencing formulation (exact) is shown in Fig. 5. The profiles are compared at two different times during the evolution. Note that good agreement exists between the variational solution and the finite differencing solution. In table 1 the execution time for the variational formulation is compared to the the time taken by the IMSL routine DPDES to obtain the solution for the same number of time steps. The calculations were performed on a VAX 3800 computer system. Note the factor of 10 gain in computer time of the variational formulation over the finite differencing scheme for the usual 40 grid points used in most applications. Note also that the CPU times for the two methods are comparable when the differencing routine is employed with 5 radial grid points. The radial profiles obtained via the variational and the 5 radial grid finite differencing methods are compared in Fig. 6. Note that interpolation is required in order to extract the complete solution and thus the 5 radial grid point finite differencing method does not provide adequate resolution.

6.4 Coupled equations.

Since our goal is to apply the variational formulation to realistic plasma transport equations it is important to generalize the method to include

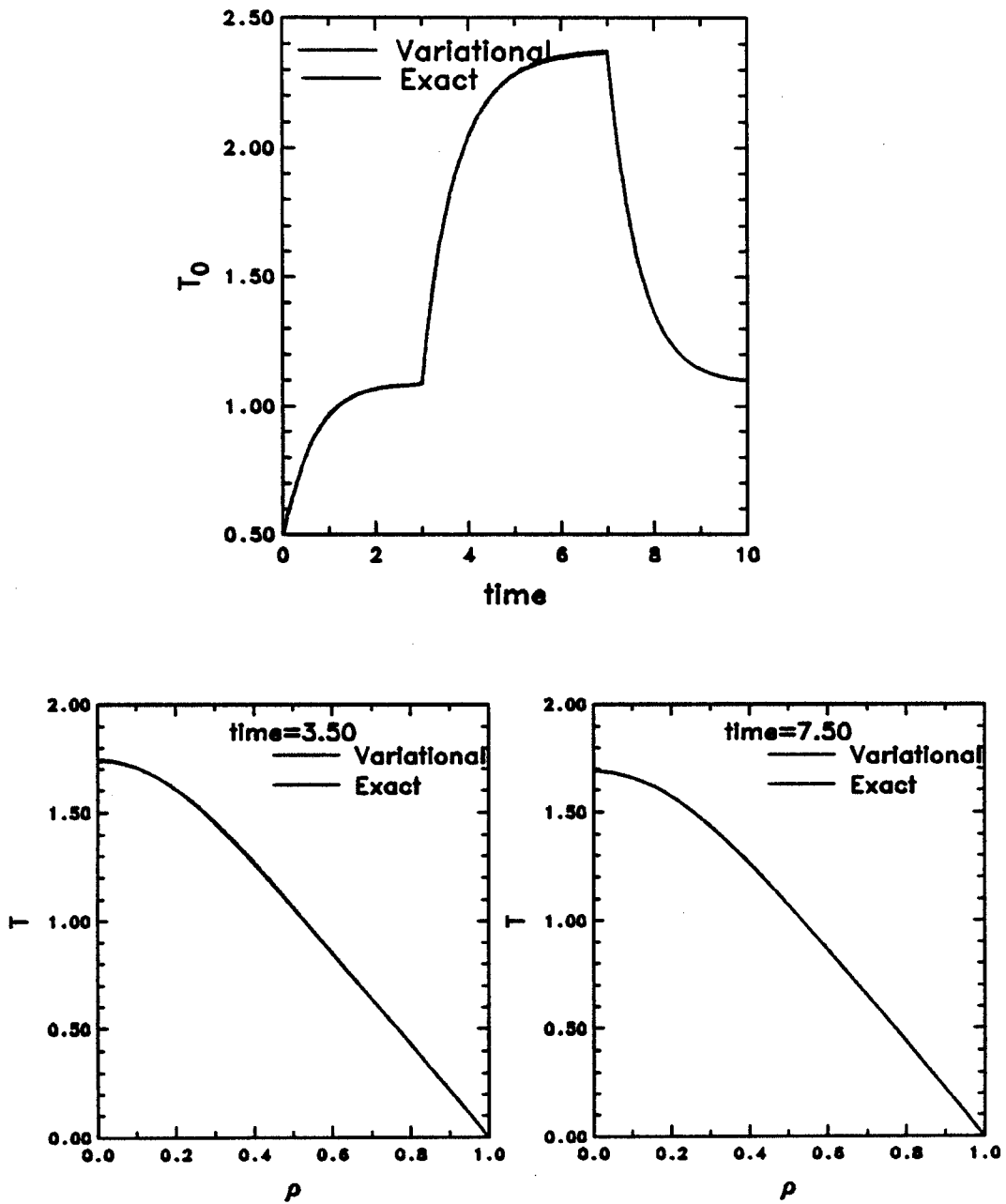


Figure 5: Comparison of the results obtained from the variational and the finite differencing formulation of the non-linear problem characterized by a centrally peaked heat pulse. Note that the time evolution of the peak temperature, shown in (a), is in excellent agreement for the two methods. In (b), and (c), the profiles are compared at times $t = 3.5$ and $t = 7.5$ respectively and there appears to be excellent agreement between the two methods.

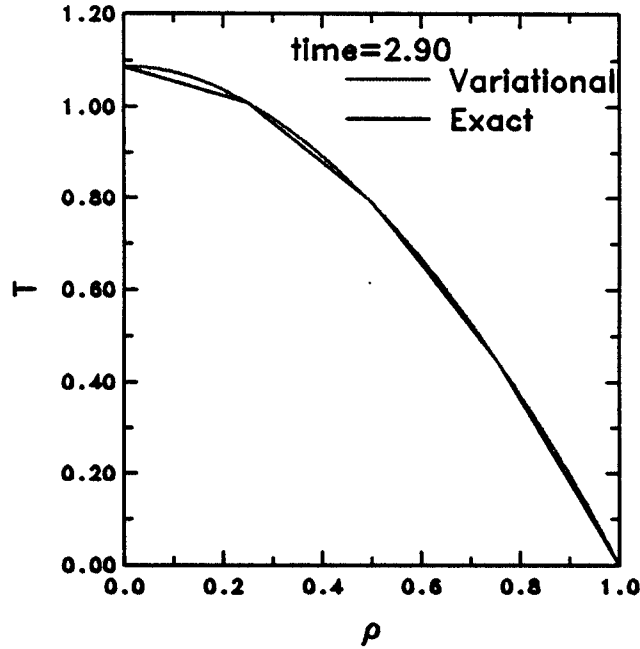


Figure 6: Comparison of the profile obtained by a five radial grid point finite differencing method and the variational formulation.

coupled transport equations. The following system of equations is considered

$$\frac{\partial T_e}{\partial t} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \left[\kappa_e(T_e, T_i, \rho, t) \frac{\partial T_e}{\partial \rho} \right] + S_e(T_e, T_i, \rho, t) \quad (69)$$

$$\frac{\partial T_e(0, t)}{\partial \rho} = 0 \quad (70)$$

$$T_e(1, t) = 0 \quad (71)$$

$$T_e(\rho, 0) = f_e(\rho) \quad (72)$$

$$\frac{\partial T_i}{\partial t} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \left[\kappa_i(T_e, T_i, \rho, t) \frac{\partial T_i}{\partial \rho} \right] + S_i(T_e, T_i, \rho, t) \quad (73)$$

$$\frac{\partial T_i(0, t)}{\partial \rho} = 0 \quad (74)$$

$$T_i(1, t) = 0 \quad (75)$$

$$T_i(\rho, 0) = f_i(\rho) \quad (76)$$

Following the formalism presented in section 4 the Lagrangian of the above system of equations is

$$\mathcal{L} = \int_0^1 \rho d\rho \left[T_e \frac{\partial \widehat{T}_e}{\partial t} + \frac{1}{2} \widehat{\kappa}_e \left(\frac{\partial T_e}{\partial \rho} \right)^2 - I_e \right] \quad (77)$$

$$+ \int_0^1 \rho d\rho \left[T_i \frac{\partial \widehat{T}_i}{\partial t} + \frac{1}{2} \widehat{\kappa}_i \left(\frac{\partial T_i}{\partial \rho} \right)^2 - I_i \right] \quad (78)$$

where

$$I_e \equiv \int_{\widehat{T}_e}^{T_e} S_e dT_e \quad (79)$$

$$I_i \equiv \int_{\widehat{T}_i}^{T_i} S_i dT_i \quad (80)$$

By assuming trial functions of the form given by Eq. (33) for T_e , and T_i

$$T_e = T_{e0}(1 - \rho^2) \exp[\alpha_1 \rho^2 + \alpha_2 \rho^4] \quad (81)$$

$$T_i = T_{i0}(1 - \rho^2) \exp[\beta_1 \rho^2 + \beta_2 \rho^4] \quad (82)$$

the equations to be solved can be written in matrix form

$$\vec{V} = \vec{M}^{-1} \vec{X} \quad (83)$$

where \vec{V} is a column vector with components

$$\vec{V} = \begin{bmatrix} \dot{T}_{e0} \\ \dot{\alpha}_1 \\ \dot{\alpha}_2 \\ \dot{T}_{i0} \\ \dot{\beta}_1 \\ \dot{\beta}_2 \end{bmatrix} \quad (84)$$

\vec{M} is a 6×6 matrix,

$$\vec{M} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 & 0 \\ A_{12} & A_{22} & A_{23} & 0 & 0 & 0 \\ A_{13} & A_{23} & A_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & B_{11} & B_{12} & B_{13} \\ 0 & 0 & 0 & B_{12} & B_{22} & B_{23} \\ 0 & 0 & 0 & B_{13} & B_{23} & B_{33} \end{bmatrix} \quad (85)$$

In the above matrix the elements labeled A_{ij} correspond to T_e , and the elements labeled B_{ij} correspond to T_i , and are given by

$$A_{11} = \frac{1}{T_{e0}^2} \int_0^1 T_e^2 \rho d\rho \quad (86)$$

$$A_{12} = \frac{1}{T_{e0}} \int_0^1 T_e^2 \rho^3 d\rho \quad (87)$$

$$A_{13} = \frac{1}{T_{e0}} \int_0^1 T_e^2 \rho^5 d\rho \quad (88)$$

$$A_{22} = \int_0^1 T_e^2 \rho^5 d\rho \quad (89)$$

$$A_{23} = \int_0^1 T_e^2 \rho^7 d\rho \quad (90)$$

$$A_{33} = \int_0^1 T_e^2 \rho^9 d\rho \quad (91)$$

$$B_{11} = \frac{1}{T_{i0}^2} \int_0^1 T_i^2 \rho d\rho \quad (92)$$

$$B_{12} = \frac{1}{T_{i0}} \int_0^1 T_i^2 \rho^3 d\rho \quad (93)$$

$$B_{13} = \frac{1}{T_{i0}} \int_0^1 T_i^2 \rho^5 d\rho \quad (94)$$

$$B_{22} = \int_0^1 T_i^2 \rho^5 d\rho \quad (95)$$

$$B_{23} = \int_0^1 T_i^2 \rho^7 d\rho \quad (96)$$

$$B_{33} = \int_0^1 T_i^2 \rho^9 d\rho \quad (97)$$

The elements of the column vector \vec{X} are

$$X_1 = \frac{1}{T_{e0}} \int_0^1 \left[-\kappa_e \left(\frac{\partial T_e}{\partial \rho} \right)^2 + S_e T_e \right] \rho d\rho \quad (98)$$

$$X_2 = \int_0^1 \left[-\kappa_e \frac{\partial T_e}{\partial \rho} \frac{\partial}{\partial \rho} (\rho^2 T_e) + S_e T_e \rho^2 \right] \rho d\rho \quad (99)$$

$$X_3 = \int_0^1 \left[-\kappa_e \frac{\partial T_e}{\partial \rho} \frac{\partial}{\partial \rho} (\rho^4 T_e) + S_e T_e \rho^4 \right] \rho d\rho \quad (100)$$

$$X_4 = \frac{1}{T_{i0}} \int_0^1 \left[-\kappa_i \left(\frac{\partial T_i}{\partial \rho} \right)^2 + S_i T_i \right] \rho d\rho \quad (101)$$

$$X_5 = \int_0^1 \left[-\kappa_e \frac{\partial T_i}{\partial \rho} \frac{\partial}{\partial \rho} (\rho^2 T_i) + S_i T_i \rho^2 \right] \rho d\rho \quad (102)$$

$$X_6 = \int_0^1 \left[-\kappa_e \frac{\partial T_i}{\partial \rho} \frac{\partial}{\partial \rho} (\rho^4 T_i) + S_i T_i \rho^4 \right] \rho d\rho \quad (103)$$

By assuming

$$\kappa_e = 0.1 \exp[\rho^2] \quad (104)$$

$$\kappa_i = 0.5 \exp[\rho^2] \quad (105)$$

$$S_e = \frac{1}{(T_e + 2.0)^{1.5}} + 5.0 \frac{T_i - T_e}{(T_e + 2.0)^{1.5}} \quad (106)$$

$$S_i = -5.0 \frac{T_i - T_e}{(T_e + 2.0)^{1.5}} \quad (107)$$

the variational solution of Eqs. (69, 73) is compared, in Fig. 7, to the “exact” solution obtained by finite differencing. The time evolution of the

Table 2: Comparison of execution times on a VAX computer for the variational and finite differencing methods for the problem of coupled non-linear transport equations.

Method		Time (sec.)
Variational		5.71
Differencing	40 grid points	39.27
Differencing	30 grid points	28.16
Differencing	20 grid points	21.37
Differencing	10 grid points	9.18
Differencing	5 grid points	6.06

central values of T_e , and T_i is shown in Fig. 7 (a), (b) respectively. Comparisons of the profiles for T_e , and T_i at time $t = 1.0$ are shown in Fig 7 (c), and (d). Table 2 shows approximate execution times, on a VAX 3800 computer system, for the variational formulation and for the finite differencing method.

7 Variational Formulation of a General System of Transport Equations.

Having developed and tested the variational formulation for a single transport equation, and for a system of two coupled transport equations the generalization of the formulation to an arbitrary number of transport equations is presented below.

The general one dimensional transport equation in cylindrical geometry is given by

$$c_j \frac{\partial U_j}{\partial t} = \sum_k \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho D_{jk} \frac{\partial U_k}{\partial \rho} \right) + S_j \quad (108)$$

where U_j are the thermodynamic variables such as temperature, density, flux, etc. The parameters c_j are various weight factors, D_{jk} are the transport coefficients, and S_j are the sources and sinks.

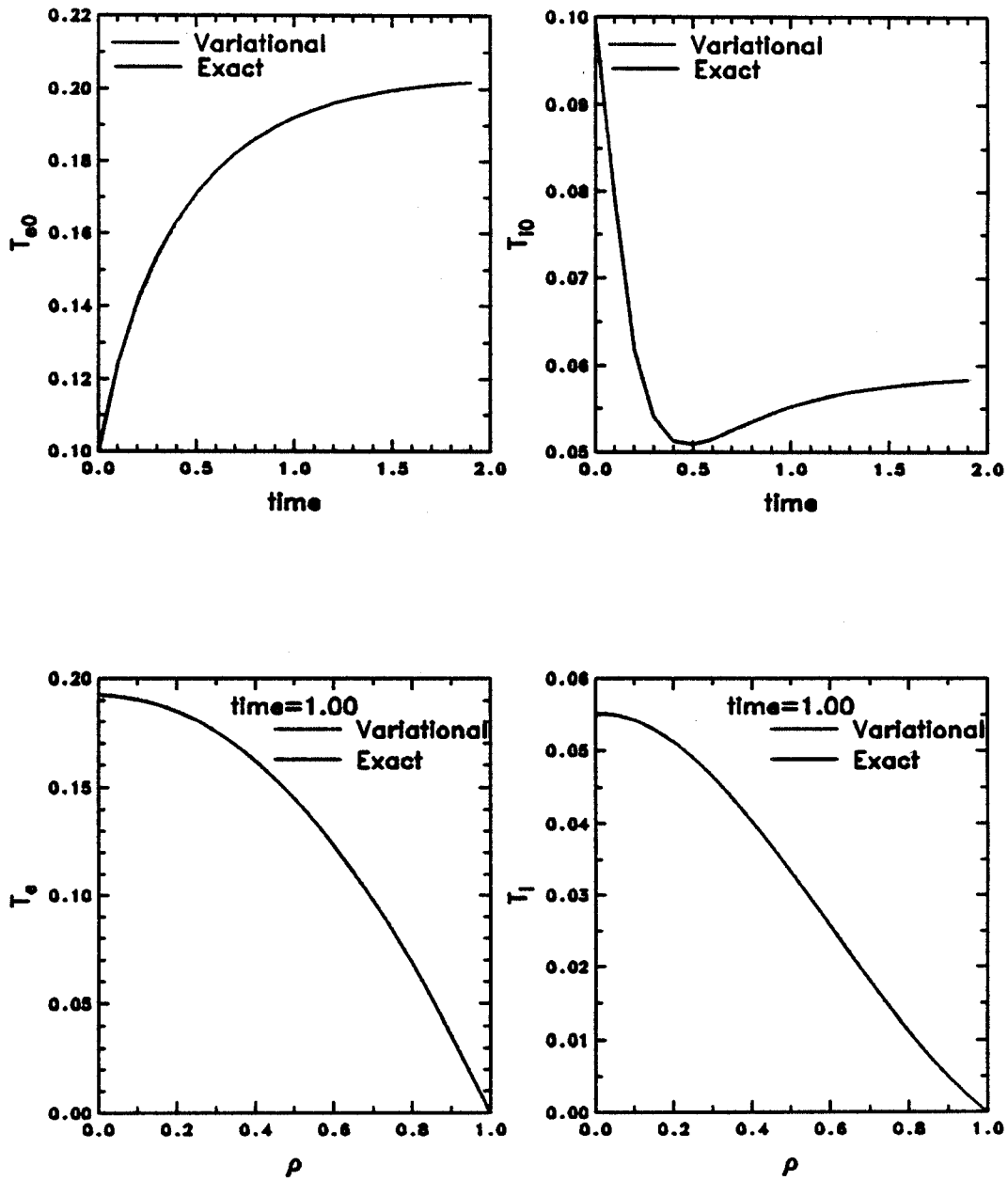


Figure 7: Comparison of the results obtained from the variational and the finite differencing formulation of a system of two coupled non-linear heat equations. The time evolution of the temperature for the two species is shown in (a), and (b). In (c), and (d) the profiles at time $t=1.0$ for the two species are compared.

$$c_j = c_j(U_1, U_2, \dots, \rho) \quad (109)$$

$$D_{jk} = D_{jk}(U_1, U_2, \dots, \rho) \quad (110)$$

$$S_j = S_j(U_1, U_2, \dots, \rho) \quad (111)$$

The initial and boundary conditions have the form

$$U_j(\rho, 0) = U_{j0} \quad \text{Initial Condition}$$

$$\frac{\partial U_j}{\partial \rho}(0, t) = 0 \quad \text{Regularity at } \rho = 0 \quad (112)$$

$$U_j(1, t) = U_{j1} \quad \text{Boundary condition at the edge}$$

The Lagrangian of Eq. (108) is given by

$$\begin{aligned} \mathcal{L} = \sum_j \int_0^1 \rho d\rho \left[N_j \frac{\partial \hat{U}_j}{\partial t} + \frac{1}{2} \sum_k \widehat{D}_{jk} \frac{\partial U_j}{\partial \rho} \frac{\partial U_k}{\partial \rho} - W_j \right] \\ - \rho \widehat{D}_{jk} \frac{\partial \hat{U}_j}{\partial \rho} U_k \end{aligned} \quad (113)$$

where in the usual fashion the functions \hat{U}_j are set equal to U_j after the variation. The parameters N_j , and W_j are given by

$$N_j = N_j(\hat{U}_1, \hat{U}_2, \dots, \hat{U}_{j-1}, U_j, \hat{U}_{j+1}, \dots, \rho) \quad (114)$$

$$W_j = W_j(\hat{U}_1, \hat{U}_2, \dots, \hat{U}_{j-1}, U_j, \hat{U}_{j+1}, \dots, \rho) \quad (115)$$

Note that only U_j is to be varied in Eqs. (114, 115). By taking the first variation of Eq. (113), and setting it equal to zero, the j^{th} component becomes

$$\frac{\partial N_j}{\partial U_j} \frac{\partial U_j}{\partial t} - \sum_k \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \left(\frac{\widehat{D}_{jk} + \widehat{D}_{kj}}{2} \right) \frac{\partial U_k}{\partial \rho} - \frac{\partial W_j}{\partial \rho} = 0 \quad (116)$$

By requiring Onsager symmetry for the matrix D (i.e. $D_{jk} = D_{kj}$), and by defining

$$N_j = \int_{\widehat{U}_j}^{U_j} c_j(\widehat{U}_{j'}, U_j, \rho) dU_j \quad j' \neq j \quad (117)$$

$$W_j = \int_{\widehat{U}_j}^{U_j} S_j(\widehat{U}_{j'}, U_j, \rho) dU_j \quad j' \neq j \quad (118)$$

the first variation of Eq. (113) yields the original equation as its Euler equation.

The Lagrangian can now be written in the matrix form

$$\begin{aligned} \mathcal{L} = \int_0^1 \rho d\rho \left[\vec{N} \cdot \frac{\partial \vec{U}}{\partial t} + \frac{1}{2} \left(\frac{\partial \vec{U}}{\partial \rho} \right)^T \cdot \widehat{\vec{D}} \cdot \left(\frac{\partial \vec{U}}{\partial \rho} \right) - \vec{W} \cdot \vec{I} \right] \\ - \rho \left(\frac{\partial \vec{U}}{\partial \rho} \right)^T \cdot \widehat{\vec{D}} \cdot \vec{U} \Big|_{\rho} = 1 \end{aligned} \quad (119)$$

where \vec{I} is the identity column vector.

This general treatment has been used to obtain solutions to the general plasma transport equations.[11] In particular the work of reference [11] includes the formulation of an $1\frac{1}{2}$ -D variational plasma transport model. A computer program called MITra has been developed which solves the plasma transport equations variationally with a large savings in the required computational effort.

8 Conclusion

The method by which variational techniques can be used to obtain solutions to the transport equations has been presented. The accuracy of the

variational formulation has been investigated in the cases for which analytic solutions exist. Also, the variational formulation was tested for accuracy and speed of execution for a single non-linear equation and for a problem of coupled non-linear equations. It is shown that accurate solutions can be obtained by employing the variational formulation with a decrease by an order of magnitude in the required computer execution time. Further reduction in the execution time can be obtained by optimizing the computation. This optimization can be obtained by precalculating certain frequently used quantities and integrals, as well as by optimizing the matrix inversion algorithm. The procedure has been extended to a set of N differential equations.

References

- [1] C. Lanczos. *The Variational principles of Mechanics*. Univ. of Toronto Press, Toronto, 1949.
- [2] H. Goldstein. *Classical Mechanics*. Addison-Wesley, Reading, Massachusetts, 1950.
- [3] R. Weinstock. *Calculus of Variations*. McGraw-Hill, New York, 1952.
- [4] I. Prigogine. Evolution Criteria Variational Properties and Fluctuations. In *Symposium on Non-Equilibrium Thermodynamics*, chapter 1, pages 3–16. University of Chicago Press, 1965.
- [5] P.M. Morse and H. Feshbach. *Methods of Theoretical Physics*. McGraw-Hill, New York, 1953.
- [6] I. Prigogine. *Bull. Acad. Belg. Cl. Sci.*, 31:600, 1954.
- [7] L. D. Landau and e. M. Lifshitz. *Statistical Physics*. Addison-Wesley, Reading, Mass., 1958.
- [8] P. Glansdorff, I. Prigogine, and D.F. Hayes. Variational properties of a viscous liquid at a nonuniform temperature. *Physics of Fluids*, 5:144–149, 1962.
- [9] I. Prigogine. *Introduction to Thermodynamics of Irreversible Processes*. Wiley, New York, second edition, 1961.
- [10] J.P. Freidberg. *Ideal Magnetohydrodynamics*. Modern Perspectives in Energy. Plenum Press, New York, 1987.
- [11] E.A. Chaniotakis. *Ignition and Burn Control Characteristics of Thermonuclear Plasmas*. PhD thesis, Massachusetts Institute of Technology, 1990.