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The F_N-Method in Kinetic Theory
I. Half-Space Problems

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ABSTRACT

The recently developed F_N-method is used to solve two half-space problems of kinetic theory: heat transfer and weak evaporation. A relatively low-order approximation gives results accurate to 6 significant figures.

I. INTRODUCTION

The F_N-method was first introduced by Siewert and Benoist[1] and Grandjean and Siewert[2] in the context of neutron transport theory. This method proved to be quite accurate even for low-order approximations[2] and thus has been extensively developed in the fields of neutron transport theory and radiative transfer. Both multi-region[3,4] and multigroup[5,6,7] problems have been solved, although the multi-group problems have been limited to down-scattering only. The only applications in kinetic theory have been to the problems of plane Poiseuille

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flow[8] and strong evaporation[9,10]. Of these, only one[10] involved the fully coupled kinetic equations which arise from the linear BGK model equation for a gas with three degrees of freedom. A method utilizing polynomial expansions of unknown surface distributions, in the spirit of the F_N method, was used by Buckner and Ferziger[11] and Loyalka and Ferziger[12].

It is the purpose of the present work to demonstrate the general method of formulation of the F_N-method for fully-coupled kinetic equations by solving two half-space problems: heat transfer and weak evaporation. Although the general method of formulation is quite similar from problem to problem, the choice of approximation is somewhat problem-dependent. As experience with the F_N method accumulates general guidelines are beginning to emerge; however one still must systematically test each candidate for a particular problem. In this paper we concentrate on half-space problems, and develop an effective approximation which we think will be useful for other half-space problems in kinetic theory.

The two problems we wish to consider have been formulated and solved by the method of elementary solutions by Siewert and Thomas[13], correcting the Wiener-Hopf results of Pao[14]. Following that formulation, we seek solutions of the coupled equations

$$\mu \frac{\partial}{\partial x} \underset{\sim}{\Psi}(x,\mu) + \underset{\sim}{\Psi}(x,\mu) = \frac{1}{\sqrt{\pi}} \underset{\sim}{Q}(\mu) \int_{-\infty}^{\infty} \tilde{\underset{\sim}{Q}}(\mu')\underset{\sim}{\Psi}(x,\mu')\exp(-\mu'^2)d\mu' , \qquad (1)$$

where $\underset{\sim}{\Psi}(x,\mu)$ is a 2-vector whose components are related to perturbations in the gas density and temperature according to

$$N(x) = \pi^{1/2} \begin{bmatrix} 1 \\ 0 \end{bmatrix}^T \int_{-\infty}^{\infty} \underset{\sim}{\Psi}(x,\mu)\exp(-\mu^2)d\mu , \qquad (2)$$

and

$$T(x) = \frac{2}{3}\pi^{1/2} \int_{-\infty}^{\infty} \begin{bmatrix} \mu^2 - \frac{1}{2} \\ 1 \end{bmatrix}^T \underset{\sim}{\Psi}(x,\mu)\exp(-\mu^2)d\mu \ . \tag{3}$$

Here $\underset{\sim}{Q}(\mu)$ is a matrix of polynomials[13], and the superscript tilde denotes the transpose operation.

For the evaporation problem, the appropriate boundary conditions are[13]

$$\underset{\sim}{\Psi}(0,\mu) = -\frac{2U}{\pi}\mu \begin{bmatrix} 1 \\ 0 \end{bmatrix} , \ \mu > 0 \ , \tag{4}$$

and

$$\lim_{x\to\infty} \frac{dN(x)}{dx} = \lim_{x\to\infty} \frac{dT(x)}{dx} = 0 \ , \tag{5}$$

where U is the downstream mass velocity.

For the heat transfer problem, we seek the solution of Eq. (1) satisfying

$$\underset{\sim}{\Psi}(0,\mu) = \underset{\sim}{0}, \quad \mu > 0 \ , \tag{6}$$

and

$$\lim_{x\to\infty} \frac{dT(x)}{dx} = -\lim_{x\to\infty} \frac{dN(x)}{dx} = 1 \tag{7}$$

After deriving the elementary solutions $\underset{\sim}{\Phi}_\alpha(\mu)$, $\underset{\sim}{\Psi}_\alpha(x,\mu)$, and $\underset{\sim}{\Phi}_\alpha(\eta,\mu)$, Kriese, Chang, and Siewert[15] have given the general solution of Eq. (1) in the form

$$\underset{\sim}{\Psi}(x,\mu) = \sum_{\alpha=1}^{2} A_\alpha \underset{\sim}{\Phi}_\alpha(\mu) + \sum_{\alpha=3}^{4} A_\alpha \underset{\sim}{\Psi}_\alpha(x,\mu)$$

$$+ \sum_{\alpha=1}^{2} \int_{-\infty}^{\infty} A_\alpha(\eta)\underset{\sim}{\Phi}_\alpha(\eta,\mu)\exp(-x/\eta)d\eta \ , \tag{8}$$

where the A_α and $A_\alpha(\eta)$ are arbitrary coefficients to be determined by the boundary conditions of the respective problems. For the evaporation problem, it can easily be determined that $\underset{\sim}{\Psi}(x,\mu)$ will satisfy the conditions of Eq. (5) if we take $A_3 = A_4 = 0$, and $A_\alpha(\eta) = 0$, $\eta < 0$, $\alpha = 1,2$. Evaluating the resulting solution at x=0, we have

$$\underset{\sim}{\Psi}(0,\mu) = \sum_{\alpha=1}^{2} A_\alpha \underset{\sim}{\Phi}_\alpha(\mu) + \sum_{\alpha=1}^{2} \int_0^\infty A_\alpha(\eta) \underset{\sim}{\Phi}_\alpha(\eta,\mu) d\eta . \tag{9}$$

II. Analysis

Using the full-range orthogonality relations of Kriese, Chang and Siewert[15], we obtain the singular integral equations

$$\int_{-\infty}^{\infty} \underset{\sim}{\tilde{X}}_\beta(\mu) \underset{\sim}{\Psi}(0,\mu) \mu\, e^{-\mu^2} d\mu = 0, \quad \beta=3,4, \tag{10}$$

and

$$\int_{-\infty}^{\infty} \underset{\sim}{\tilde{X}}_\beta(-\eta,\mu) \underset{\sim}{\Psi}(0,\mu) \mu\, e^{-\mu^2} d\mu = 0, \quad \beta=1,2. \tag{11}$$

The vectors $\underset{\sim}{X}_\beta(\mu)$ and $\underset{\sim}{X}_\beta(\eta,\mu)$ are given explicitly in Reference 15.

Since $\underset{\sim}{\Psi}(0,\mu)$ is known only for $\mu > 0$ from the boundary condition (4), we introduce the approximation

$$\underset{\sim}{\Psi}(0,-\mu) = \underset{\sim}{Q}(\mu)\Big[\underset{\sim}{C}_0 + \sum_{\alpha=1}^{N} \underset{\sim}{C}_\alpha \frac{1}{\nu_\alpha+\mu}\Big], \quad \mu > 0, \tag{12}$$

where $\underset{\sim}{Q}(\mu)$ is the same polynomial matrix used in Eq. (1), $\underset{\sim}{C}_\alpha$ are 2-vectors to be determined, and the ν_α, $0 < \nu_\alpha < \infty$, are chosen to maximize computational efficiency. It is seen that an approximation of order N involves N+1 unknown vectors $\underset{\sim}{C}_\alpha$, for a total of 2N+2 unknowns. Substituting the approximation (12) and the boundary condition (4) into Eqs.

(10) and (11) yields the equations

$$\pi^{-1/2}\begin{bmatrix}\frac{7}{2}\\ -(\frac{3}{2})^{1/2}\end{bmatrix}^T \cdot \underset{\sim}{C}_0 + \sum_{\alpha=1}^{N} \tilde{\underset{\sim}{P}}_1(\nu_\alpha)\underset{\sim}{C}_\alpha = 0, \tag{13}$$

$$\pi^{-1/2}\begin{bmatrix}-(\frac{2}{3})^{1/2}\\ 6\end{bmatrix}^T \cdot \underset{\sim}{C}_0 + \sum_{\alpha=1}^{N} \tilde{\underset{\sim}{P}}_2(\nu_\alpha)\underset{\sim}{C}_\alpha = -\frac{5U}{\pi}, \tag{14}$$

and

$$\tilde{\underset{\sim}{R}}_\beta(\eta)\underset{\sim}{C}_0 + \sum_{\alpha=1}^{N} \tilde{\underset{\sim}{R}}_\beta(\eta,\nu_\alpha)\underset{\sim}{C}_\alpha = -\begin{bmatrix}1\\0\end{bmatrix}^T \frac{2U}{\pi}\underset{\sim}{S}_\beta(\eta), \quad \beta = 1,2. \tag{15}$$

Here

$$\underset{\sim}{P}_\beta(\nu_\alpha) = \int_0^\infty \tilde{\underset{\sim}{Q}}(\mu)\ \underset{\sim}{X}_{\beta+2}(-\mu)\mu e^{-\mu^2}\frac{d\mu}{\nu_\alpha+\mu}, \tag{16}$$

$$\underset{\sim}{R}_\beta(\eta) = \int_0^\infty \tilde{\underset{\sim}{Q}}(\mu)\ \underset{\sim}{X}_\beta(-\eta,-\mu)\mu e^{-\mu^2}d\mu, \tag{17}$$

$$\underset{\sim}{R}_\beta(\eta,\nu_\alpha) = \int_0^\infty \tilde{\underset{\sim}{Q}}(\mu)\ \underset{\sim}{X}_\beta(-\eta,-\mu)\mu e^{-\mu^2}\frac{d\mu}{\nu_\alpha+\mu}, \tag{18}$$

and

$$\underset{\sim}{S}_\beta(\eta) = \int_0^\infty \underset{\sim}{X}_\beta(-\eta,\mu)\mu^2 d\mu, \tag{19}$$

for $\beta = 1$ and 2.

The integrals in Eqs. (16-19) can all be reduced to combinations of the basic integral

$$I(\xi) = \int_0^\infty \frac{e^{-\mu^2}}{\mu+\xi}\,d\mu,$$

however, the details are rather tedious and are given elsewhere[16]. Eq. (15) evaluated at N values of $\eta=\eta_j$, along with Eqs. (13) and (14) yield a system of 2N + 2 algebraic equations for the $\underset{\sim}{C}_\alpha$, $\alpha = 0,\ldots,N$, which can be solved straightforwardly using standard methods. Once these coefficients are computed, the expansion coefficients A_α, $A_\alpha(\eta)$, $\alpha=1,2$ used in Eq. (9) are available from the aforementioned full-range orthogonality[15]:

$$A_\alpha = \int_{-\infty}^{\infty} \tilde{\underset{\sim}{X}}_\alpha(\mu)\underset{\sim}{\Psi}(0,\mu)\mu\exp(-\mu^2)d\mu, \quad \alpha = 1,2 , \tag{20}$$

and

$$A_\alpha(\eta) = \int_{-\infty}^{\infty} \tilde{\underset{\sim}{X}}_\alpha(\eta,\mu)\underset{\sim}{\Psi}(0,\mu)\mu\exp(-\mu^2)d\mu , \quad \alpha = 1,2 . \tag{21}$$

This leads immediately to values of the density and temperature profiles through[11]

$$T(x) = \pi(2/3)^{1/2}A_1 + \pi^{1/2}\int_0^\infty A_1(\eta)\exp(-\eta^2 - x/\eta)d\eta , \tag{22}$$

and

$$N(x) = \pi A_2 + \pi^{1/2}\int_0^\infty A_2(\eta)\exp(-\eta^2 - x/\eta)d\eta . \tag{23}$$

The other quantities of interest are the macroscopic density and temperature jumps, c_1 and d_1, and the microscopic density and temperature jumps, γ_1 and δ_1, respectively, defined by[14]

$$\lim_{x\to\infty} N(x) = -2Uc_1 , \qquad \lim_{x\to\infty} T(x) = -2Ud_1 ,$$
$$N(0) = -2U\gamma_1 , \qquad T(0) = -2U\delta_1 . \tag{24}$$

For the heat-transfer problem, the boundary conditions (7) require

$$A_3 = -\frac{1}{\pi}\left(\frac{3}{2}\right)^{1/2}, \tag{25a}$$

$$A_4 = \frac{1}{\pi}, \tag{25b}$$

and

$$A_\alpha(\eta) = 0, \quad \eta < 0 . \tag{25c}$$

For this case, full-range orthogonality applied to the general solution (9) and incorporating Eq. (25c) yields the singular integral equations

$$\int_{-\infty}^{\infty} \tilde{X}_\beta(\mu)\Psi(0,\mu)\mu\, e^{-\mu^2} d\mu = A_\beta, \quad \beta = 3,4, \tag{26}$$

and

$$\int_{-\infty}^{\infty} \tilde{X}_\beta(-\eta,\mu)\Psi(0,\mu)\mu\, e^{-\mu^2} d\mu = 0, \quad \beta = 1,2. \tag{27}$$

We now approximate $\Psi(0,-\mu)$ in the form

$$\Psi(0,-\mu) = Q(\mu)\left[C_0 - \frac{\mu}{\pi}\begin{bmatrix} -\left(\frac{3}{2}\right)^{1/2} \\ 1 \end{bmatrix} + \sum_{\alpha=1}^{N} C_\alpha \frac{1}{\nu_\alpha+\mu}\right]. \tag{28}$$

Inserting this approximation along with the boundary condition (6) into Eqs. (26) and (27), we find the equations

$$\pi^{-1/2}\begin{bmatrix} \frac{7}{2} \\ -\left(\frac{3}{2}\right)^{1/2} \end{bmatrix}^T C_0 + \sum_{\alpha=1}^{N} \tilde{P}_1(\nu_\alpha)C_\alpha = \frac{5}{2\pi}\left(\frac{3}{2}\right)^{1/2}, \tag{29}$$

$$\pi^{-1/2}\begin{bmatrix} -\left(\frac{2}{3}\right)^{1/2} \\ 6 \end{bmatrix}^T C_0 + \sum_{\alpha=1}^{N} \tilde{P}_2(\nu_\alpha)C_\alpha = -\frac{5}{2\pi} \tag{30}$$

and

$$\tilde{R}_\beta(\eta)C_0 + \sum_{\alpha=1}^{N} \tilde{R}_\beta(\eta,\nu_\alpha)C_\alpha = \frac{1}{\pi}\int_0^\infty \tilde{X}_\beta(-\eta,-\mu)Q(\mu)\mu^2\exp(-\mu^2)d\mu \begin{bmatrix} -(\frac{3}{2})^{1/2} \\ 1 \end{bmatrix},$$

$$\beta = 1,2. \tag{31}$$

We note that these equations differ from Eqs. (13-15) only on their respective right-hand sides.

The numerical procedure is the same as for the evaporation problem. The resulting expressions for the density and temperature profiles now are[13]

$$N(x) = \pi A_2 - x + \pi^{1/2} \int_0^\infty A_2(\eta)\exp(-\eta^2 - x/\eta)d\eta , \tag{32}$$

and

$$T(x) = \pi(\tfrac{2}{3})^{1/2} A_1 + x + \pi^{1/2} \int_0^\infty A_1(\eta)\exp(-\eta^2 - x/\eta)d\eta. \tag{33}$$

The macroscopic density and temperature jumps[14] may be determined from these equations according to

$$\lim_{x\to\infty} [N(x) + x] = -c_2, \quad \lim_{x\to\infty} [T(x) - x] = d_2 ,$$
$$N(0) = -\gamma_2, \qquad T(0) = \delta_2 . \tag{34}$$

III. Numerical Results

We chose the ν_α , $\alpha = 1,2,\ldots,N$, in the F_N-approximations, Eqs. (12) and (28), to be the N positive zeros of the Hermite polynomial of degree 2N. The linear algebraic equations (13-15) for the evaporation problem, and (29-31) for the heat transfer problem were then solved by standard techniques. Since the resulting temperature and density

Table I. Evaporation Problem

N	Temperature $x=0$, δ_1	Temperature $x\to\infty$, d_1	Density $x=0$, γ_1	Density $x\to\infty$, c_1
2	0.204629	0.223222	0.661150	0.842701
4	0.204798	0.223374	0.661082	0.842620
6	0.204800	0.223379	0.661099	0.842628
8	0.204797	0.223378	0.661109	0.842633
10	0.204795	0.223377	0.661116	0.842637
12	0.204794	0.223377	0.661118	0.842638
14	0.204793	0.223376	0.661120	0.842640
16	0.204792	0.223376	0.661122	0.842641
18	0.204791	0.223376	0.661124	0.842642
20	0.204791	0.223376	0.661125	0.842642
22	0.204791	0.223375	0.661125	0.842642
24	0.204791	0.223376	0.661126	0.842642
26	0.204791	0.223376	0.661126	0.842643
28	0.204790	0.223375	0.661127	0.842643
30	0.204790	0.223375	0.661128	0.842644
Converged Results	0.204790	0.223375	0.661128	0.842644
Exact[13]	0.204789	0.223375	0.661130	0.842645

Table II. Heat Transfer Problem

N	Temperature		Density	
	$x=0,\ \delta_2$	$x\to\infty,\ d_2$	$x=0,\ \gamma_2$	$x\to\infty,\ c_2$
2	0.850307	1.30011	0.393898	0.742053
4	0.853215	1.30249	0.396276	0.744059
6	0.853428	1.30266	0.396470	0.744214
8	0.853471	1.30269	0.396515	0.744246
10	0.853503	1.30271	0.396583	0.744286
12	0.853499	1.30270	0.396569	0.744279
14	0.853503	1.30270	0.396569	0.744278
16	0.853505	1.30271	0.396568	0.744277
18	0.853506	1.30271	0.396568	0.744278
20	0.853507	1.30271	0.396569	0.744278
22	0.843409	1.30271	0.396569	0.744278
24	0.853507	1.30271	0.396570	0.744277
26	0.853511	1.30271	0.396570	0.744279
28	0.853513	1.30272	0.396571	0.744279
30	0.853512	1.30272	0.396570	0.744278
Converged Results	0.853513	1.30272	0.396571	0.744279
Exact[13]	0.853515	1.30272	0.396572	0.744279

profiles agreed with the exact results[13] to six significant figures for $N \leq 30$, we chose not to tabulate them here.

The rate of convergence of the F_N method for these problems is evident in Tables I and II, where we present computed values of the various slip coefficients, by taking $U = \frac{1}{2}$, as the F_N order is increased. In general, convergence is faster for quantities evaluated at $x \to \infty$ (e.g. c_1, d_1, c_2, and d_2) than for quantities evaluated at $x=0$ (δ_1, γ_1, δ_2, γ_2). This is expected since in the limit of large x the integral terms disappear in Eqs. (22,23) and (32,33).

IV. Conclusions

The chosen F_N approximation for the fully coupled kinetic equations produces excellent results for modest computational effort; 6-figure accuracy is achieved for $20 \leq N \leq 30$, and 4 figures for $N \leq 10$. Based on this success, we next intend to investigate problems in finite media, such as parallel-plates heat transfer and evaporation. Our goal is to be able to solve problems for which exact analysis in unavailable, such as heat transfer and evaporation in binary mixtures.

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References

1. C. E. Siewert and P. Benoist, Nucl. Sci. Eng. 69, 156 (1979).

2. P. Grandjean and C. E. Siewert, Nucl. Sci. Eng. 69, 161 (1979).

3. R. D. M. Garcia and C. E. Siewert, Nucl. Sci. Eng. 76, 53 (1980).

4. R. D. M. Garcia and C. E. Siewert, J. Comput. Phys. 50, 181 (1983).

5. C. E. Siewert and P. Benoist, Nucl. Sci. Eng. 78, 311 (1981).

6. R. D. M. Garcia and C. E. Siewert, Nucl. Sci. Eng. 78, 315 (1981).

7. R. D. M. Garcia and C. E. Siewert, J. Comput. Phys. 46, 237 (1982).

8. C. E. Siewert, R. D. M. Garcia, and P. Grandjean, J. Math. Phys. 21, 2760 (1980).

9. S. K. Loyalka, C. E. Siewert, and J. R. Thomas, Jr., Z. angew. Math. Phys. 32, 745 (1981).

10. C. E. Siewert and J. R. Thomas, Jr., Z. angew. Math. Phys. 33, 202 (1982).

11. J. K. Buckner and J. H. Ferziger, Phys. Fluids 9, 2315 (1966).

12. S. K. Loyalka and J. H. Ferziger, Phys. Fluids 10, 1833 (1967).

13. C. E. Siewert and J. R. Thomas, Jr., Phys. Fluids 16, 1557 (1973).

14. Y. P. Pao, Phys. Fluids 14, 1340 (1971).

15. J. T. Kriese, T. S. Chang and C. E. Siewert, Int. J. Engng Sci. 12, 441 (1974).

16. D. Valougeorgis, Ph.D. Dissertation, Virginia Polytechnic Institute and State University, Blacksburg, Virginia (1985).

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