The Use of Implicit Monte Carlo Radiation Transport with Hydrodynamics and Compton Scattering

J. A. Fleck, Jr.

RECEIVED

DEC 09 1996

OSTI

March, 1971

This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the Laboratory.

Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract W-7405-ENG-48.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

lln

MASTER

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or 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 trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or 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 the University of California, and shall not be used for advertising or product endorsement purposes.

This report has been reproduced
directly from the best available copy.

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831
Prices available from (615) 576-8401, FTS 626-8401

Available to the public from the
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd.,
Springfield, VA 22161

Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract W-7405-ENG-48.

DISCLAIMER

**Portions of this document may be illegible
in electronic image products. Images are
produced from the best available original
document.**

Lawrence Radiation Laboratory

UNIVERSITY OF CALIFORNIA

LIVERMORE

THE USE OF IMPLICIT MONTE CARLO RADIATION
TRANSPORT WITH HYDRODYNAMICS AND COMPTON SCATTERING

J. A. Fleck, Jr.

March, 1971

THE USE OF IMPLICIT MONTE CARLO RADIATION
TRANSPORT WITH HYDRODYNAMICS AND COMPTON SCATTERING

J. A. FLECK, JR.

March, 1971

INTRODUCTION

The purpose of this note is to show that the combination of implicit radiation transport and hydrodynamics, Compton scattering, and any other energy transport or exchange mechanism can be simply carried out by a "splitting" procedure. This means that the contributions to material energy exchange can be reckoned separately for hydrodynamics, radiation transport without scattering, Compton scattering, plus any other possible energy exchange mechanism. The radiation transport phase of the calculation would of course be implicit and would be carried out in exactly the manner described in UCRL-7294¹, but the hydrodynamics and Compton portions would not, leading to possible time step controls. In any case, the time step restrictions which occur on radiation transfer due to large Planck mean absorption cross-sections would not occur.

EQUATIONS

The equations which govern the radiation transport are

$$\frac{1}{c} \frac{\partial I_v}{\partial t} + \mu \frac{\partial I_v}{\partial x} + (\sigma_v + \sigma_v^C) I_v = \int \sigma^C(\mu', v' \rightarrow \mu, v) I(\mu', v') \frac{v}{v'} d\mu' dv' + \frac{1}{2} c \sigma_v B_v$$

1a

$$\frac{\partial u_m}{\partial \tau} = \iiint \sigma_\nu I_\nu d\nu d\mu - c \int \sigma_\nu E_\nu d\nu + S \quad (1b)$$

In Equation (1a) σ_ν is the frequency dependent absorption cross-section, σ_ν^C is the total frequency dependent Compton scattering cross-section, and $\sigma^C(\mu'; \nu' \rightarrow \mu, \nu)$ is the cross-section for Compton scattering from direction μ' and frequency ν' to direction μ and frequency ν . In Eq.(1a) stimulated or induced scattering contributions have been neglected.² In Eq. (1b) u_m represents the matter energy density and S represents the rate of energy exchange to the matter from all sources other than absorption of radiation, e.g. pdv work and Compton exchange. For the sake of definiteness we shall assume that the Compton energy exchange remains from the previous cycle and that the hydrodynamics and pdv work are computed at the beginning of the current cycle. These restrictions will be removed later.

In order to derive the implicit radiation transfer equations we write Eq. (1a) as b

$$\frac{\partial u_r}{\partial \tau} = \beta \left\{ \iiint \sigma_\nu I_\nu d\nu d\mu - \alpha_p u_r \right\} + \beta S \quad (2)$$

where

$$u_r = a T^4, \quad (3a)$$

and

$$\beta = \frac{\partial u_r}{\partial u_m} = \frac{4aT^3}{b}. \quad (3b)$$

with

$$b(T) = \frac{\partial u_m}{\partial T} \quad (3c)$$

Integrating Eq. (2) from time t^n to time t^{n+1} we get

$$u_r^{n+1} - u_r^n = \int_{t^n}^{t^{n+1}} dt \beta \iint \sigma_v \bar{I}_v dv d\mu - c \int_{t^n}^{t^{n+1}} dt \beta \sigma_p u_r + \int_{t^n}^{t^{n+1}} dt \beta S \quad (4a)$$

$$u_r^{n+1} - u_r^n = \beta \Delta t \left\{ \iint \sigma_v \bar{I}_v dv d\mu - c \bar{\sigma}_p \left[\alpha u_r^{n+1} + (1-\alpha) \beta \bar{S} \Delta t + (1-\alpha) u_r^n \right] \right\} + \beta \bar{S} \Delta t \quad (4b)$$

In going from Eq. (4a) to Eq. (4b) we have represented the average value of u_r under the integral sign in the second right hand member of (4a) as

$$\bar{u}_r = \alpha u_r^{n+1} + (1-\alpha) \left[u_r^n + \beta \bar{S} \Delta t \right] \quad (4c)$$

instead of by means of the more accurate expression (at least when $\alpha=1/2$)

$$\bar{u}_r = \alpha u_r^{n+1} + (1-\alpha) u_r^n, \quad (4d)$$

which was used in UCRL-72924. Expression (4c) is employed for formal reasons which will be apparent shortly. In the completely implicit case ($\alpha=1$) Eqs.(4c) and (4d) are identical.

We now make the identification

$$u_r^{n*} = u_r^n + \beta S \Delta t \quad (5)$$

where, for convenience, average bars have been dropped. Here the superscript n^* signifies a time between t^n and t^{n+1} . Solving Eq.(4b) for u_r^{n+1} now yields

$$u_r^{n+1} = \frac{\beta \Delta t}{1 + \alpha \beta c \Delta t \sigma_p} \int \bar{I}_v \sigma_v dv d\mu + \left[\frac{1 - (1-\alpha) \beta c \Delta t \sigma_p}{1 + \alpha \beta c \Delta t \sigma_p} \right] u_r^{n*} \quad (6)$$

This is like Eq.(1.8) of UCRL-72924 but with the source term eliminated.

If $\bar{u}_r$ is calculated from

$$\bar{u}_r = \alpha u_r^{n+1} + (1-\alpha) u_r^{n*}, \quad (7)$$

and substituted into the transport equation (1a) the result is

$$\begin{aligned} \frac{1}{c} \frac{\partial I_v}{\partial x} + \mu \frac{\partial I_v}{\partial x} + (\sigma_v + \sigma_v^C) I_v = \frac{1}{2} \sigma_v b_v \left[\frac{\alpha \beta c \Delta t}{1 + \alpha \beta c \Delta t \sigma_p} \right] \iint \sigma_v' I_{v'} dv' d\mu' \\ + \int \sigma^C(\mu', v' \rightarrow \mu, v) I(\mu', v') \frac{v}{v'} d\mu' dv' \quad (8) \\ + \frac{1}{2} \frac{c \sigma_v b_v u_r^{n*}}{1 + \alpha \beta c \Delta t \sigma_p}, \end{aligned}$$

where b_v represents a normalized Planck spectrum, and any reference to the source term S is now contained in u_r^{n*} . The interpretation of (8) is that the effective absorption cross-section is now

$$\sigma_{va} = \sigma_v \left[\frac{1}{1 + \alpha \beta c \Delta t \sigma_p} \right], \quad (9)$$

the effective scattering cross-section due to absorption and reemission is

$$\sigma_{vs} = \sigma_v \left[\frac{\sigma_p \alpha \beta c \Delta t}{1 + \alpha \beta c \Delta t \sigma_p} \right], \quad (10)$$

and the total effective scattering cross-section is

$$\sigma_s^T = \sigma_v^C + \sigma_{vs} \quad (11)$$

Equation (8) is assumed valid from time t^n to t^{n+1} . Thus we now integrate Eq.(8) over angle and frequency to obtain a conservative form of the matter energy density equation. We obtain

$$\frac{1}{c} \frac{\partial}{\partial t} \iint dv d\mu I_v + \frac{\partial F}{\partial x} = - \frac{\partial u_m}{\partial t} + S = - \left(\frac{\partial u_m}{\partial t} \right)_C - \iint dv d\mu \sigma_v I_v + \left(\frac{\alpha \beta c \Delta t \sigma_p}{1 + \alpha \beta c \Delta t \sigma_p} \right) \iint dv d\mu \sigma_v I_v + \frac{c \sigma_p u_r^{n*}}{1 + \alpha \beta c \Delta t \sigma_p} \quad (12)$$

In Eq.(12) $(\partial u_m / \partial t)_C$ represents the energy exchange rate from radiation to matter due to Compton scattering and is given by

$$\left(\frac{\partial u_m}{\partial t} \right)_C = \int d\mu dv \int \sigma(\mu, \nu \rightarrow \mu', \nu') I(\nu, \mu) dv' d\mu' - \int d\mu dv \int \sigma(\mu', \nu' \rightarrow \mu, \nu) I(\nu, \mu') \frac{\nu}{\nu'} dv' d\mu' \quad (13)$$

Combining terms in Eq.(12) gives

$$\frac{\partial u_m}{\partial t} = S + \left(\frac{\partial u_m}{\partial t} \right)_C + \frac{1}{1 + \alpha \beta c \Delta t \sigma_p} \iint dv d\mu \sigma_v I_v - \frac{c \sigma_p u_r^{n*}}{1 + \alpha \beta c \Delta t \sigma_p} \quad (14)$$

Replacing $\partial u_m / \partial t$ by $b(T)(\partial T / \partial t)$ and integrating Eq.(14) from t^n to t^{n+1} gives

$$T^{n+1} = T^n + b^{-1} \left\{ S \Delta t + \left(\frac{\partial u_m}{\partial t} \right)_C \Delta t + \frac{1}{1 + \alpha \beta c \Delta t \sigma_p} \int_{t^n}^{t^{n+1}} dt \iint dv d\mu \sigma_v I_v - \frac{c \sigma_p \Delta t u_r^{n*}}{1 + \alpha \beta c \Delta t \sigma_p} \right\} \quad (15)$$

We can define

$$T^{n*} = T^n + b^{-1} S \Delta t \quad (16)$$

If the updating of temperature indicated in Eq.(16) is carried out first, and a radiation source function is calculated from

$$u_r^{n*} = a(T^{n*})^4 = a(T^n + b^{-1} S \Delta t)^4, \quad (17)$$

then

$$u_r^{n*} = a T^{n4} + 4(T^n)^3 b^{-1} S \Delta t + O((\Delta t)^2) = u_r^n + \beta S \Delta t + O(\Delta t^2) \quad (18)$$

Thus u_r^{n*} calculated with the updated temperature T^{n*} from Eq.(16) agrees with u_r^{n*} as defined by Eq.(5), to first order in Δt . Therefore, we can safely do the temperature update (16) first and then calculate an emission source function for the radiation transfer part of the calculation afterward.

By our original assumption, S includes the Compton energy exchange from the previous time cycle. To be completely consistent the energy contribution

$$\left(\frac{\partial u_m}{\partial t} \right)_C \Delta t \quad (19)$$

ought to be carried forward to the next time cycle. However, it is obvious that the Compton temperature update can be considered to be made equally well at the end of the current cycle as well as at the beginning of the next cycle. The only difference will be in the value of $b(T)$ employed.³ The order of the hydrodynamic update, whether made before or after the radiation update, is also immaterial. The radiation update for Compton energy exchange and emission-absorption balance is made simultaneously at the end of the radiation transport calculation for the cycle.

SUMMARY

Let us assume for the sake of definiteness that the hydrodynamics is performed first during a given time cycle. Next, the temperature is updated by means of

$$T^{n*} - T^n = b^{-1} \Delta t \left(\frac{\partial u_m}{\partial t} \right)_{\text{Hydro}} \quad (20)$$

One then calculates

$$u_r^{n*} = a(T^{n*})^4 \quad (21a)$$

Although one could also use

$$u_r^{n*} = a(T^n)^4 + \beta \left(\frac{\partial u_m}{\partial t} \right)_{\text{Hydro}} \quad (21.b)$$

if convenient. One also calculates

$$f = \frac{1}{1 + \alpha \beta c \Delta t \sigma_p} \quad , \quad (21.c)$$

$$\sigma_{va} = f \sigma_v \quad , \quad (21.d)$$

$$\sigma_{vs} = (1-f) \sigma_v \quad . \quad (21.e)$$

The following transport equation is then solved with the radiation solution being advanced from t^n to t^{n+1}

$$\begin{aligned} \frac{1}{c} \frac{\partial I_v}{\partial t} + \mu \frac{\partial I_v}{\partial x} + (\sigma_{va} + \sigma_{vs} + \sigma_v^c) I_v &= \int \sigma^c(\mu', v' \rightarrow \mu, v) I(\mu', v') \frac{v}{v'} dv' d\mu' \\ &+ \frac{1}{2} (1-f) (\sigma_v b_v / \sigma_p) \iint \sigma_v I_v dv' d\mu' + \frac{1}{2} f c \sigma_v b_v u_r^{n*} \end{aligned} \quad (22)$$

The final temperature update is given by

$$\begin{aligned} T^{n+1} &= T^{n*} + b^{-1} f \left\{ \int_{t^n}^{t^{n+1}} dt \iint \sigma_v I_v dv d\mu - c \Delta t \sigma_p u_r^{n*} \right. \\ &+ \int_{t^n}^{t^{n+1}} dt \int d\mu dv \int \sigma(\mu, v \rightarrow \mu', v') I(v, \mu) dv' d\mu' \\ &\left. - \int_{t^n}^{t^{n+1}} dt \int d\mu dv \int \sigma(\mu', v' \rightarrow \mu, v) I(v', \mu') \frac{v}{v'} dv' d\mu' \right\} \end{aligned} \quad (23)$$

where the first integral in Eq.(23) represents the cumulative effective absorption of radiation during a time cycle, and the second pair of integrals represents the accumulated energy transferred between radiation and matter through Compton scattering for the cycle. When a Compton

scattering takes place, the photon's energy and frequency are appropriately changed, and the energy exchanged between radiation and matter is tallied for the appropriate zone.

If desired, the radiation calculation could be performed first, and the hydrodynamics last, in which case u_r^n should replace u_r^{n*} , T^{n*} replace T^{n+1} and T^n replace T^{n*} in Eq.(23). The hydrodynamics update would give

$$T^{n+1} = T^{n*} + b^{-1} \Delta t \frac{\partial u_m}{\partial t} \text{Hydro} \quad (24)$$

REFERENCES AND FOOTNOTES

1. UCRL-72924 "An Implicit Monte Carlo Scheme for Calculating Time and Frequency Dependent Nonlinear Radiation Transport."
2. It is possible, if desired, to take into account induced effects in a zeroth moment approximation as is now done in completely explicit calculations. The ensuing arguments used here will not be affected by this procedure.
3. From the point of view of effective energy conservation it is actually superior to work with the matter energy density variable u_m , to advance this quantity as a result of the various mechanisms of energy transfer and deposition, and then at the end of a time cycle to determine temperature as a function of u_m by means of a table lookup.

DISTRIBUTION

INTERNAL

C. Barnett
H. Barnett
R. Bentley
N. Byrne
E. Canfield
G. Chapline
A. Cole
G. Cooper
G. Corman
P. Crowley
D. Cummings
R. Debar
D. Eardley
F. Eby
P. Eltgroth
J. Fleck
E. Garelis
R. Gelinas
L. Germain
P. Giles
A. Goldberg
E. Goldberg
W. Grasberger
W. Grayson
D. Hall
R. Howerton
C. Hendrickson
J. Hughes
N. Keeler
R. Kidder

J. LeBlanc
W. Loewe
W. Lokke
S. Maxon
M. May
R. McLean
L. Milton
P. Moulthrop
R. Nelson
W. Noh
J. Nuckolls
S. Perkins
E. Plechaty
A. Porter
D. Post
J. Ramus
W. Schulz
W. Shaw
C. Tarter
E. Teller
K. Trigger
P. Vajk
T. Wainwright
J. Wilson
A. Winslow
W. Zagotta
W. Zink

Technical Information Dept. (2 copies)
Theoretical Files (3 copies)