Adjoint-based Sensitivity Analysis for High-Energy Density Radiative Transfer using Flux-Limited Diffusion

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Abstract

Uncertainty quantification and sensitivity analyses are a vital component for predictive modeling in the sciences and engineering. The adjoint approach to sensitivity analysis requires solving a primary system of equations and a mathematically related set of adjoint equations. The information contained in the equations can be combined to produce sensitivity information in a computationally efficient manner. In this work, sensitivity analyses are performed on systems described by flux-limited radiative diffusion using the adjoint approach. The sensitivities computed are shown to agree with standard perturbation theory and require significantly less computational time. The adjoint approach saves the computational cost of one forward solve per sensitivity, making the method attractive when multiple sensitivities are of interest.

Keywords: Flux limited diffusion, radiative diffusion, sensitivity analysis, adjoint.

1. Introduction

The adjoint approach to performing sensitivity analyses is an efficient method for identifying parameters that have the greatest influence on a particular quantity of interest (QOI). The adjoint method requires formulation of a second

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5 problem, mathematically related to the forward system of equations, and uses
the solution to obtain sensitivity information. This approach allows multiple
sensitivities to be computed by solving the forward and adjoint equations once,
and evaluating inner products for each sensitivity. This is computationally ef-
ficient compared to the perturbation approach to finding sensitivities, which
10 requires solving the forward problem twice per perturbed parameter. The sen-
sitivity is then found by dividing the change in the QOI by the change in the
perturbed parameter.

The main disadvantage of the adjoint approach is that can quickly become mem-
ory intensive [1], [2]. The forward and adjoint solutions, along with parameter
15 values, must be stored for all time, and at all spatial locations, in order to
compute the sensitivities. For high fidelity, transient calculations the memory
demand can rapidly exceed that available on standard computers. Typically,
writing and reading to files is required, or a subset of information is stored and
the solutions are recomputed from these checkpoints [3].

20 The methodology for deriving an adjoint system of coupled differential equations
is well documented [4], [5], [6]. In this work, the adjoint equations are derived
for a system of coupled partial differential equations describing radiative flux-
limited diffusion. Approximations to complex expressions that result from the
non-linear flux-limited diffusion model are shown not to introduce significant
25 error when computing sensitivities. The resulting system of adjoint equations
are linear, thus it takes less computational time to perform a full sensitivity
analysis using the adjoint approach than it takes to compute a single sensitivity
using the perturbation method.

2. Adjoint-based sensitivity analysis

An adjoint-based sensitivity analysis is performed on a system described by
flux-limited radiative diffusion with material temperature feedback. The evolu-
tion of the forward system is described by a set of coupled partial differential

equations [7], [8], [9]:

$$\begin{aligned} \frac{1}{c} \frac{\partial \phi}{\partial t} - \nabla \cdot D \nabla \phi &= S - \kappa \rho (\phi - acT^4), \\ \rho C_v \frac{\partial T}{\partial t} &= \kappa \rho (\phi - acT^4), \end{aligned} \quad (1)$$

where $\phi = \phi(r, t)$ is the scalar intensity with units of GJ/cm²ns, $T = T(r, t)$ is the temperature in keV, c is 29.98 cm/ns, a is 0.01372 GJ/cm³-keV⁴, S is an external volumetric source, κ is the opacity, ρ is the density, C_v is the specific heat, and D is the flux-limited diffusion coefficient. Note that the solutions, ϕ and T , depend implicitly on the material constants and the diffusion coefficient.

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Flux-limited diffusion coefficients are designed to correct for non-physical results related to the speed of propagation of information. In the diffusion approximation, the current is given by the expression:

$$J = -D \nabla \phi. \quad (2)$$

The approximation is inaccurate where the gradient of the scalar intensity is large; flux-limited diffusion coefficients prevent the current from exceeding physical values in such regions. The Larsen coefficient is used in this work [10]:

$$D = \left((3\kappa\rho)^n + \left(\frac{1}{\phi} |\nabla \phi| \right)^n \right)^{-1/n}. \quad (3)$$

When the gradient of the scalar intensity is small, this reduces to the standard diffusion coefficient; when the gradient is large, the second term in the denominator dominates, thus preventing the current from exceeding the scalar intensity. Typically n is chosen to be two, but it can be adjusted such that the diffusion solution agrees more closely with transport calculations [11].

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To derive the equations for the adjoint scalar intensity, $\phi^\dagger$, and the adjoint temperature, $T^\dagger$, we use the Lagrangian approach to form the sensitivity expression. First, the differential equations are combined to form the operator F :

$$F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} = \begin{pmatrix} \dot{\phi}/c - f(\phi, T) \\ \dot{T} - g(\phi, T) \end{pmatrix} = 0, \quad (4)$$

with

$$\begin{aligned} f(\phi, T) &= \nabla \cdot D\nabla\phi - \kappa\rho(\phi - acT^4) + S, \\ g(\phi, T) &= \frac{\kappa\rho}{\rho C_v}(\phi - acT^4). \end{aligned} \quad (5)$$

Following the work of Stripling [3] and Stripling, Anitescu, and Adams [12], to find the adjoint system for the coupled set of equations, a Lagrangian is formed:

$$\mathcal{L} = \int [\langle Q \rangle - \langle \lambda, F \rangle] dt, \quad (6)$$

where the angular brackets denote integrals over all space and $\langle Q \rangle$ is the quantity of interest. The integral over time is taken from t_0 to t_f . The operator F is defined to be zero, thus the sensitivities of $\langle Q \rangle$ and $\mathcal{L}$ are equivalent. To derive the expression for the sensitivity, the functional derivative of the Lagrangian is taken with respect to θ using the chain rule:

$$\frac{\partial \mathcal{L}}{\partial \theta} = \int \left[\langle Q \rangle_\theta + \langle Q \rangle_x x_\theta - \frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle \dot{x}_\theta - \frac{\partial}{\partial x} \langle \lambda, F \rangle x_\theta - \frac{\partial}{\partial \theta} \langle \lambda, F \rangle \right] dt. \quad (7)$$

In this equation, $x = (\phi \ T)^T$, the subscripts denote partial derivatives, $\dot{x}$ is the time derivative of x , and λ is an undetermined two component Lagrange multiplier. Using integration by parts, the integral can be rewritten as:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \theta} &= \left[-\frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle x_\theta \right]_{t_0}^{t_f} + \int \left[\langle Q_\theta \rangle - \frac{\partial}{\partial \theta} \langle \lambda, F \rangle \right] dt \\ &\quad + \int \left[\langle Q_x \rangle + \frac{d}{dt} \left(\frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle \right) - \frac{\partial}{\partial x} \langle \lambda, F \rangle \right] x_\theta dt, \end{aligned} \quad (8)$$

The only term in the above expression that cannot be computed directly is x_θ , the derivative of the solution vector with respect to θ . If this term was known, the adjoint approach would not be necessary as the sensitivity could be computed by direct differentiation of the QOI.

The adjoint equations are defined to be the conditions that are imposed on $\lambda \equiv (\phi^\dagger \ T^\dagger)^T$ such that the integrand of the final term is eliminated. Thus, the adjoint equations are given by the expression:

$$\left[-\frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle x_\theta \right]_{t_0}^{t_f} + \langle Q_x \rangle + \frac{d}{dt} \left(\frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle \right) - \frac{\partial}{\partial x} \langle \lambda, F \rangle = 0. \quad (9)$$

Note that the first term in (9) includes the sensitivity of the initial conditions to the parameter θ . This term can be included if known; in the work that follows it is simply assumed that the sensitivity of the initial conditions is not of interest and the term is taken to be zero; this assumption is not necessary in general. However, the value of x_θ at the final time is not known, and must be eliminated by imposing appropriate terminal conditions on the adjoint variables. The resulting system of adjoint equations evolve backward in time, with the terminal condition:

$$\lambda(t_f) = 0. \quad (10)$$

Physically, the terminal condition states that events occurring beyond the final time step do not influence the adjoint solution [3], [13].

To summarize, the forward system of equations (Eq. (1)) are solved provided initial conditions and the adjoint system of equations (Eq. (9)) are solved by imposing terminal conditions (Eq. (16)). The forward and adjoint solutions can then be used to evaluate the sensitivity of the QOI with respect to any parameter, θ , by evaluating Eq. (11):

$$\frac{\partial \mathcal{L}}{\partial \theta} = \int \left[\langle Q_\theta \rangle - \frac{\partial}{\partial \theta} \langle \lambda, F \rangle \right] dt. \quad (11)$$

The QOI for the following examples is the time integrated absorption, $\mathcal{A}$, in particular regions, thus:

$$\langle Q \rangle = \int \rho \kappa \phi \, dV, \quad (12)$$

where the spatial integral is taken over the volume of interest. The expressions for F and $\langle Q \rangle$ are substituted into equation (9), and the system is split into its constituent components. The result is a set of coupled equations for the adjoint scalar intensity and the adjoint temperature:

$$\begin{aligned} -\frac{1}{c} \frac{\partial \phi^\dagger}{\partial t} - \nabla \cdot (D \nabla \phi^\dagger) + \kappa \rho \phi^\dagger &= \kappa \rho + \frac{\kappa}{C_v} T^\dagger, \\ -\frac{\partial T^\dagger}{\partial t} &= -\frac{4\kappa \rho T^3}{\rho C_v} T^\dagger + \frac{\partial}{\partial T} (\kappa \rho \phi) - \frac{\partial}{\partial T} (\kappa \rho \phi \phi^\dagger). \end{aligned} \quad (13)$$

The final expression for the sensitivity of the absorption, $\mathcal{A}$, with respect to

an arbitrary parameter θ is given by:

$$\frac{\partial \mathcal{A}}{\partial \theta} = \left[\frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle x_\theta \right]_{t_0} + \int \left[\langle Q_\theta \rangle - \frac{\partial}{\partial \theta} \langle \lambda, F \rangle \right] dt. \quad (14)$$

50 2.1. Sensitivity Examples

In this study the primary quantity of interest is the total absorption within particular volumes:

$$\mathcal{A} = \int \int \kappa \rho \phi \, dV \, dt,$$

where the integration over time is taken from t_0 to t_f and the spatial integration is taken over a region of interest. When computing sensitivities, a few complicated derivatives must be evaluated. For example, when computing the sensitivity of the absorption with respect to the opacity, the following derivative appears in the final term of equation (14):

$$\frac{\partial}{\partial \kappa} \left(-\nabla \cdot \left(\left\{ (3\kappa\rho)^n + \left(\frac{1}{\phi} |\nabla \phi| \right)^n \right\}^{-1/n} \nabla \phi \right) \right). \quad (15)$$

The flux-limited form of the diffusion coefficient complicates the spatial derivative. To avoid performing this derivative analytically, a second-order centered finite difference approximation is employed. For a particular direction in Cartesian geometry, the expression above is estimated by:

$$-\frac{\partial}{\partial \kappa} \left(\frac{\partial}{\partial r} D \frac{\partial \phi}{\partial r} \right)_i \approx -\frac{1}{\Delta r} \left(\left(\frac{\partial D}{\partial \kappa} \frac{\partial \phi}{\partial r} \right)_{i+1/2} - \left(\frac{\partial D}{\partial \kappa} \frac{\partial \phi}{\partial r} \right)_{i-1/2} \right), \quad (16)$$

where Δr is the discretization step size for coordinate r and $i \pm 1/2$ subscripts denote where on the discretized domain the functions should be evaluated. The derivative of the diffusion coefficient with respect to the opacity is calculated analytically. Similar approximations are made for the sensitivity of the absorption

55 with respect to the parameter n in the diffusion coefficient.

2.2. Numerical Methods

The adjoint equations are derived in their continuous form, however in practice they are solved numerically. The discretization scheme must be chosen such

that the properties of the adjoint equations are preserved. Many Runge-Kutta
60 schemes have been shown to retain the properties of the continuous adjoint
equations, such as the implicit Euler and fourth order Runge-Kutta discretiza-
tions [3]. Furthermore, these schemes possess symmetries that allow for inte-
gration forward and backward in time without requiring modification to the
algorithm. For the forward equations an initial condition is supplied; for the
65 adjoint equations a terminal condition is specified.

In this work, the implicit Euler discretization is used to solve the forward and
adjoint systems of equations. The equation for the radiation scalar intensity
becomes nonlinear with use of the flux-limited diffusion coefficient. In order to
define a unique adjoint operator, the diffusion coefficient is linearized by lag-
70 ging ϕ one time step in the forward solve, and using the known forward scalar
intensity in the expression for D to solve the adjoint equations.

The nonlinear forward temperature equation is also solved implicitly; the solu-
tion is converged when the relative L-2 norm of the solutions ϕ and T changes
less than 10^{-8} between iterations. The adjoint system is solved using similar
75 convergence criteria.

3. Crooked Pipe Example

Sensitivity analyses are carried out for a 2-D cylindrical crooked pipe prob-
lem [14]. The geometry is defined in Figure 1; a radiation source turned on
at $t = 0$ is located at the left inlet of the optically thin material. The pa-
80 rameters for this problem are summarized in Table 1. The problem defined by
Graziani [14] is modified by replacing the incoming scalar intensity boundary
condition at the left inlet with an open boundary condition and a volumetric
source. The source strength is $0.1 \text{ GJ/cm}^3\text{ns}$ distributed throughout the first
two cells along the horizontal axis and from $r=0 \text{ cm}$ to $r=0.5 \text{ cm}$.

Table 1: Parameter values for cylindrical crooked pipe example.

Parameter	Value
$dr=dz$	0.05 (cm)
dt	0.01 (ns)
ρ (thin)	0.01 (g/cm ³)
ρ (thick)	10 (g/cm ³)
C_v (thin)	0.05 (GJ/g/keV)
C_v (thick)	0.05 (GJ/g/keV)
κ	20 (cm ² /g)
T_{initial}	0.005 (keV)
S	0.1 (GJ/cm ³ ns)

85 Figure 1 illustrates the pipe geometry with two regions of interest indicated for the sensitivity analysis.

Figure 1: Crooked pipe geometry with regions 1 and 2 noted. The three points are locations for the time evolution figures. The pipe is symmetric about the bottom horizontal axis.

We first consider the case of constant opacity. Under this assumption, the adjoint temperature equation has a null solution; the material properties do not depend explicitly on temperature, thus the derivatives in equation (13) vanish.

90 For illustrative purposes, Figures 2 and 3 depict the forward and adjoint scalar intensity at 10 ns. The forward solution is plotted in terms of radiation temperature, defined by $\phi = acT_R^4$. Figures 4 and 5 illustrate the time dependence

of the solutions at the three points numbered in Fig. 1.

Figure 2: Radiation temperature at 10 ns for temperature independent opacity.

Figure 3: Adjoint scalar intensity at 10 ns. The quantity of interest is the absorption in region 1, indicated on Figure 1.

The quantities of interest are the energy absorption within the entire system
 95 and within regions 1 and 2, indicated in Figure 1. The perturbed parameters
 include the source, opacity, densities, and the exponent n in the diffusion coefficient.
 The adjoint approach is compared to the traditional perturbation theory
 result; the method in which the problem is solved twice to compute a single
 sensitivity. The resulting sensitivities are summarized in Table 2. In the table,
 100 the “forward” method refers to the perturbation result; the “adjoint” method
 refers to the adjoint sensitivity. The absorption is computed by integrating $\phi \cdot$
 $\kappa \rho$ over the region and time period of interest.

The direct and adjoint methods give the same order of importance for the
 sensitivities, and differ in magnitude by less than 10%. Thus, the finite differ-
 105 ence approximations to the derivatives of the QOI do not introduce a significant
 amount of error; mesh refinement could further improve the approximation if

Table 2: Forward and adjoint sensitivities of energy absorption with temperature-independent opacity, integrated over the first 10 ns.

Total volume; absorption= 0.59596 GJ			
θ	Forward Sensitivity	Adjoint Sensitivity	% Difference
κ	2.4629	2.3487	4.864
ρ_{thin}	2.46293	2.3041	6.449
ρ_{thick}	-0.0012	-0.00112	6.656
S	5.9533	5.9853	0.537
n	0.1353	0.1368	1.097

Region 1; absorption = 0.00487 GJ			
θ	Forward Sensitivity	Adjoint Sensitivity	% Difference
κ	-0.0844	-0.0905	6.772
ρ_{thin}	-0.000752	-0.000729	3.059
ρ_{thick}	-0.08434	-0.08095	4.019
S	0.04407	0.04069	8.3076
n	-0.01339	-0.0127	8.3076

Region 2; absorption = 0.00172 GJ			
θ	Forward Sensitivity	Adjoint Sensitivity	% Difference
κ	-0.0595	-0.0552	7.925
ρ_{thin}	-0.0603	-0.0566	6.202
ρ_{thick}	-0.00077	-0.00073	4.262
S	0.0162	0.0154	4.964
n	0.0000497	0.000049	1.515

Figure 4: Time evolution of the radiation temperature at locations indicated in Figure 1.

Figure 5: Time evolution of the adjoint scalar intensity at locations indicated in Figure 1. The quantity of interest is the total absorption in the system.

necessary. The adjoint method is only advantageous if it requires less computational time than the perturbation approach. The time to complete the forward solve is 31.6 s; it would take 63.2 s to compute a single sensitivity using the
110 perturbation method. The time to complete the adjoint solve is 16.7 s, with an additional 2.7 s to compute five sensitivities. The adjoint approach requires about 23% less time than the perturbation method when computing only a single sensitivity. When multiple sensitivities are of interest, the time savings with the adjoint approach becomes more significant. The simplifications due
115 to temperature independent material properties contribute to the time savings;

the adjoint system is reduced to a single equation that is simpler to solve than the coupled forward solutions.

To illustrate the advantage of the adjoint approach for a more realistic system, temperature dependent material properties are considered. The crooked pipe problem is solved again with a temperature dependent opacity [15] [16]:

$$\kappa = \frac{\kappa_0}{T^3}, \quad (17)$$

where κ_0 is the value in Table 1. The resulting sensitivities are summarized in Table 3.

120 In this more complicated problem the adjoint method quantifies the sensitivities with less than 10% error and predicts the correct order of importance for the parameters. With temperature dependent opacities, the forward system takes 37.03 s to solve; thus a single sensitivity computed via the perturbation method can be obtained in 74.06 s. The adjoint temperature is no longer zero,
125 thus the set of coupled adjoint equations is solved; this task takes 17.1 s, and the five inner products for the sensitivities take 2.8 s to compute. Even in the more complicated case of temperature dependent opacity, multiple sensitivities can be computed in less computational time than a single sensitivity can be calculated via the perturbation approach.

130 4. Conclusions

The adjoint equations for a flux-limited radiative diffusion model are derived and used to perform sensitivity analyses. Due to the nonlinearity of the diffusion coefficient, the sensitivity expressions contain cumbersome derivatives; proposed finite difference approximations to these derivatives are shown to not
135 introduce significant error. The adjoint method is particularly advantageous when the sensitivity of a quantity of interest with respect to multiple variables is needed. For the crooked pipe example, the forward system is composed of two coupled nonlinear partial differential equations. Solving the forward system iteratively requires more computational time than the adjoint equations, which

Table 3: Forward and adjoint sensitivities of energy absorption with temperature dependent opacity, integrated over the first 10 ns.

Total volume; absorption = 269.4 GJ			
θ	Forward Sensitivity	Adjoint Sensitivity	% Difference
κ	1.167	1.496	1.520
ρ_{thin}	5.1724	5.5147	6.619
ρ_{thick}	1.625	1.511	7.044
S	5.8557	6.0491	3.303
n	-0.0377	-0.0382	0.964

Region 1; absorption = 20.87 GJ			
θ	Forward Sensitivity	Adjoint Sensitivity	% Difference
κ	0.10455	0.101	3.518
ρ_{thin}	$< 10^{-10}$	$< 10^{-10}$	0
ρ_{thick}	0.01045	0.0109	4.253
S	$< 10^{-10}$	$< 10^{-10}$	0
n	0.0000206	0.000022	4.571

Region 2; absorption = 7.215 GJ			
θ	Forward Sensitivity	Adjoint Sensitivity	% Difference
κ	0.03612	0.03527	2.433
ρ_{thin}	1.0×10^{-7}	1.05×10^{-7}	5.00
ρ_{thick}	0.0361	0.0333	7.965
S	0.0000197	0.00002	1.407
n	-1.5×10^{-7}	-1.6×10^{-7}	6.25

are a set of linear coupled equations. The complete adjoint analysis for five sensitivities requires less computational time than two forward solves required to compute a single sensitivity, and quantifies sensitivities without significant error. The methodology presented in this work could readily be applied to transport and radiation hydrodynamics. The adjoint equations can be derived using the Lagrangian approach presented; it is expected that the adjoint method will be computationally efficient when two or more sensitivities are of interest. The transport equations are more complicated to solve since the operator is not self-adjoint, however it will be easier to impose non-homogeneous boundary conditions to consider a wider variety of realistic problems.

5. Acknowledgment

This material is based upon work supported by the Department of Energy, National Nuclear Security Administration, under Award Number DE-NA0002376.

References

- [1] J. M. Restrepo, G. K. Leaf, A. Griewank, Circumventing storage limitations in variational data assimilation studies, *SIAM Journal on Scientific Computing* 19 (5) (1998) 1586–1605.
- [2] A. Sandu, D. N. Daescu, G. R. Carmichael, T. Chai, Adjoint sensitivity analysis of regional air quality models, *Journal of Computational Physics* 204 (1) (2005) 222 – 252.
- [3] H. F. Stripling, Adjoint-based uncertainty quantification and sensitivity analysis for reactor depletion calculations, Ph.D. dissertation, Texas A&M University (2013).
- [4] Y. Cao, S. Li, L. Petzold, R. Serban, Adjoint sensitivity analysis for differential algebraic equations: The adjoint DAE system and its numerical solution, *SIAM J Computational Applied Mathematics* 24 (2003) 1076–1089.

- [5] R. Hartmann, Adjoint consistency analysis of discontinuous Galerkin discretizations, *SIAM J Numerical Analysis* 37 (2000) 2671–2696.
- [6] A. Sandu, On the properties of Runge-Kutta discrete adjoints, *Lec. Notes in Comp. Science* 3994 (2006) 550–557.
- [7] P. N. Brown, D. E. Shumaker, C. S. Woodward, Fully implicit solution of large-scale non-equilibrium radiation diffusion with high order time integration, *Journal of Computational Physics* 204 (2005) 760–783.
- [8] R. G. McClarren, J. G. Wohlbiere, Solutions for ion- electron- radiation coupling with radiation and electron diffusion, *JQSRT* 112 (2011) 119–130.
- [9] R. L. Bowers, J. R. Wilson, *Numerical Modeling in Applied Physics and Astrophysics*, Jones and Bartlett, Boston MA, 1991.
- [10] G. L. Olson, L. H. Auer, M. L. Hall, Diffusion, P_1 , and other approximate forms of radiation transport, *JQSRT* 64 (2000) 619–634.
- [11] R. G. McClarre, T. K. Lane, A flux-limited diffusion method for simulating radiative shocks, *Trans. Am. Nucl. Soc.* 107 (2012) 557.
- [12] H. F. Stripling, M. Anitescu, M. L. Adams, A generalized adjoint framework for sensitivity and global error estimation in time-dependent nuclear reactor simulations, *Ann. Nucl. Energy* 52 (2012) 47–58.
- [13] G. Bell, S. Glasstone, *Nuclear Reactor Theory*, Litton Educational Publishing, Inc., New York, New York, 1970.
- [14] J. L. F. Graziani, The crooked pipe test problem, *Tech. rep.*, Lawrence Livermore National Laboratory (2000).
- [15] T. K. Lane, R. G. McClarren, New self-similar radiation-hydrodynamics solutions in the high-energy density, equilibrium diffusion limit, *New Journal of Physics* 15 (9) (2013) 095013.

- [16] A. Petschek, R. Williamson, J. W. Jr., Penetration of radiation with constant driving temperature, Tech. rep., Los Alamos Scientific Laboratory, Los Alamos, NM (1960).