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DIFFERENCE EQUATIONS FOR PLANE THERMAL ELASTICITY

by

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ABSTRACT

Difference equations for the displacement components of a heated, inhomogeneous, orthotropic material are obtained from a variational principle. Including boundary terms, the matrix of the resulting linear system of equations is positive semi-definite, a property which assures solution by many iterative techniques. The equations are solved for an infinite hollow cylinder of isotropic material in which the temperature varies inversely with the radius, whose inner surface is stress free, and whose outer surface is fixed.

INTRODUCTION

For many problems in plane thermal elasticity which cannot be treated by classical analysis, a numerical method of general applicability consists of replacing the linear differential equations and boundary conditions by linear difference equations. The matrix of the system of linear equations obtained by this direct differencing has usually such a complex structure that the choice of a successful method for solving the system is extremely difficult. In this paper it is shown that the uncertainties of direct differencing can be avoided by deriving the difference equations from a variational principle. For a wide class of thermal elasticity problems, the variational approach yields a linear system with a positive semi-definite matrix, which permits iterative methods to be used with confidence.

The use to which a code based on the variational difference equations was to be put required that the basic equations describe anisotropic, inhomogeneous materials in multiply connected regions. A formulation of the thermal elasticity problem in terms of the displacement vector met these requirements as well as allowing boundary conditions of all types to be imposed in a simple manner. The differential equations and boundary conditions in terms of displacement components are derived by the variation method in the first section of this report. The second part contains a discussion of the stress-strain relation for orthotropic materials, a type of anisotropic substance of sufficient generality for the purposes of the code. The third part is a derivation of difference equations from the variational principle. The last section contains a comparison of an example calculation with the exact solution for the stresses and displacement in an infinite hollow cylinder of isotropic material in which the temperature varies inversely with radius.

I. THE BASIC DIFFERENTIAL EQUATIONS

For thermal stress problems a variational principle based on the Helmholtz free energy is a convenient means of obtaining both the differential equations and the difference equations for the displacement components.

The free energy F is assumed to be a function of the temperature T and the strain tensor $e_{ij}(i_{,j} = 1,2,3)$. From the combined first and second laws of thermodynamics for isothermal processes, the rate of change of the free energy equals the negative of the rate at which work W is being done by the stresses σ_{ij}:

$$\frac{dF}{dt} = -\frac{dW}{dt} = \sigma_{ij}\frac{de_{ij}}{dt}.* \qquad \text{(I 1)}$$

From the assumption of the dependence of F on T and e_{ij}, it is evident that

*All vectors and tensors will be referred to a rectangular cartesian coordinate system. The summation convention for repeated indices will be employed; e.g.,

$$a_{ij}b_{ik} = a_{1j}b_{1k} + a_{2j}b_{2k} + a_{3j}b_{3k}.$$

$$\sigma_{ij} = \left.\frac{\partial F}{\partial e_{ij}}\right)_T . \tag{I 2}$$

Consider the following variational principle for the case of no body forces:

$$\delta \int_V F dV - \int_{S'} T_i' \,\delta u_i dS = 0, \tag{I 3}$$

where the variations of the displacement components u_i are carried out isothermally and T_i' are stress vector components prescribed on a part of the surface S'. Integration by parts and the use of Green's formula yields

$$\int_S T_i \,\delta u_i \,dS - \int_{S'} T_i' \,\delta u_i \,dS - \int_V \sigma_{ij,j} \,\delta u_i dV = 0.* \tag{I 4}$$

The surface integral is split as follows:

$$\int_S T_i \,\delta u_i \,dS = \int_d T_i \,\delta u_i \,dS + \int_{Sy} T_i \,\delta u_i \,dS + \int_{S'} T_i' \,\delta u_i \,dS. \tag{I 5}$$

The first integral is over that part of surface where the displacements are specified and vanishes with the δu_i appropriate there. The second integral, over a symmetry boundary on which no work is done, also vanishes. The third part is cancelled by the corresponding term in (I 4). Thus the Equation (I 4) reduces to

---

* $\sigma_{ij,j} \equiv \frac{\partial \sigma_{ij}}{\partial x_j}$

$$\int_V \sigma_{ij,j}\, \delta u_i \, dV = 0. \tag{I 6}$$

For suitable functions σ_{ij} and arbitrary δu_i, we obtain by standard arguments the equilibrium equations,

$$\sigma_{ij,j} = 0. \tag{I 7}$$

The boundary conditions are the natural conditions for surface tractions,

$$T_i = T_i'(\alpha,\beta),$$

(α,β, are surface parameters); specified displacements,

$$u_i = u_i'(\alpha,\beta);$$

and symmetry conditions,

$$T_i \, \delta u_i = 0.$$

(I 8)

This last condition can be simplified by observing that for any symmetry boundary the normal component of the displacement must vanish. Since the tangential component of the displacement is still arbitrary, we can conclude that the tangential component of the stress vector must also vanish if no work is to be done on a symmetry surface. Thus the symmetry boundary conditions are mixed - - partly specified and partly natural.

The equation for displacements is next found from (I 7) by expressing the stresses σ_{ij} in terms of the displacements through a stress-strain relation. For thermal stress problems in which the temperature changes and strains are not large, the free energy can be approximated by an expansion[1]

$$F(T,e_{ij}) = F(T_o) + c_{ij}\, e_{ij}(T-T_o) + 1/2c_{ijk\ell}\, e_{ij}\, e_{k\ell}. \qquad \text{(I 9)}$$

The coefficients c_{ij} are anisotropic coefficients of thermal expansion; the $c_{ijk\ell}$ are anisotropic elastic constants. The stress from (I 2) is

$$\sigma_{ij} = c_{ij}(T-T_o) + c_{ijk\ell}\, e_{k\ell}. \qquad \text{(I 10)}$$

The equilibrium equations (I 7) may now be written in terms of the displacements,

$$(c_{ijk\ell}\, u_{k,\ell})_{,j} + [c_{ij}(T-T_o)]_{,j} = 0. \qquad \text{(I 11)}$$

The boundary condition for a specified stress vector can also be written in terms of the displacements. For an outward normal with components n_i, the stress vector components are

$$T_i = \sigma_{ij}\, n_j = c_{ij}\, n_j (T - T_o) + c_{ijk\ell}\, u_{k,\ell}\, n_j . \qquad \text{(I 12)}$$

For symmetry boundaries the normal component of the displacement must vanish,

$$u_n = u_i\, n_i = 0, \qquad \text{(I 13)}$$

and the tangential component of the stress vector must also vanish,

$$T_t = \sigma_{ij}\, n_j\, t_i = 0, \qquad \text{(I 14)}$$

where t_i is any vector lying in the tangent plane. If the material is isotropic, it can be shown that (I 13) and (I 14) together imply that

$$\frac{\partial u_t}{\partial n} = 0. \qquad \text{(I 15)}$$

If the material is anisotropic, only (I 14) can be used.

Differential Equations (I 11) plus the boundary conditions (I 8), (I 12), (I 13), and (I 14) constitute a displacement formulation of the thermal elastic problem for anisotropic materials. In the next section the equations will be specialized for a material with orthotropic symmetry and for the case of plane strain.

II. THE STRESS-STRAIN RELATIONS

Several aspects of the stress-strain relations (I 10) need to be discussed. First the form of the relation specialized for materials with orthotropic symmetry is to be determined. Also the positive definiteness of that part of the free energy quadratically dependent on the strains must be established. Finally the inequalities relating the elastic constants are to be obtained as conditions for positive definiteness.

A material is said to have orthotropic symmetry if under reflection through any of three orthogonal planes the material tensor components, $c_{ijk\ell}$, do not change their values. In a single reflection a component of a tensor has a change in sign if the index of the effected coordinate appears an odd number of times. Since all coordinates may be reflected in an orthotropic material, all components with an odd number of indices must vanish if the tensor is to be uneffected by reflection. Taking this into account and using coordinate lines which are the intersection of the symmetry planes, one has for the free energy

$$F = \tfrac{1}{2}[c_{1111}\, e_{11}^2 + c_{1122}\, e_{11}\, e_{22} + c_{2211}\, e_{22}\, e_{11} + c_{1133}\, e_{11}\, e_{33}$$

$$+ c_{3311}\, e_{33}\, e_{11} + c_{1212}\, e_{12}^2 + c_{2112}\, e_{21}\, e_{12} + c_{2121}\, e_{21}^2$$

$$+ c_{1221}\, e_{12}\, e_{21} + c_{2222}\, e_{22}^2 + c_{2233}\, e_{22}\, e_{33} + c_{3322}\, e_{33}\, e_{22}$$

$$+ c_{2323}\, e_{23}^2 + c_{3223}\, e_{32}\, e_{23} + c_{3232}\, e_{32}^2 + c_{2332}\, e_{23}\, e_{32}$$

$$+ c_{3333}\, e_{33}^2 + c_{1313}\, e_{13}^2 + c_{1331}\, e_{13}\, e_{31} + c_{3131}\, e_{31}^2$$

$$+ c_{3113}\, e_{31}\, e_{13}] + c_{11}\, e_{11}(T-T_o) + c_{22}\, e_{22}(T-T_o)$$

$$+ c_{33}\, e_{33}(T-T_o) + F(T_o). \qquad \text{(II 1)}$$

The symmetry of the strains and elastic constants reduces (II 1) to

$$F = \tfrac{1}{2}[c_{1111}\, e_{11}^2 + c_{2222}\, e_{22}^2 + c_{3333}\, e_{33}^2 + 2c_{1122}\, e_{11}\, e_{22}$$

$$+ 2c_{1133}\, e_{11}\, e_{33} + 2c_{2233}\, e_{22}\, e_{33} + 4c_{1212}\, e_{12}^2 + 4c_{1313}\, e_{13}^2$$

$$+ 4c_{2323}\, e_{23}^2] + c_{11}\, e_{11}(T-T_o) + c_{22}\, e_{22}(T-T_o) + c_{33}\, e_{33}(T-T_o)$$

$$+ F(T_o). \qquad \text{(II 2)}$$

The stresses obtained by (I 2) from (II 1) are

$$\sigma_{11} = c_{1111}\, e_{11} + c_{1122}\, e_{22} + c_{1133}\, e_{33} + c_{11}(T-T_o)$$

$$\sigma_{22} = c_{1122}\, e_{11} + c_{2222}\, e_{22} + c_{2233}\, e_{33} + c_{22}(T-T_o)$$

$$\sigma_{33} = c_{1133}\, e_{11} + c_{2233}\, e_{22} + c_{3333}\, e_{33} + c_{33}(T-T_o)$$

$$\sigma_{12} = 2c_{1212}\, e_{12}$$

$$\sigma_{13} = 2c_{1313}\, e_{13}$$

$$\sigma_{23} = 2c_{2323}\, e_{23}. \qquad \text{(II 3)}$$

These equations take a more familiar form when solved for the strains in the following manner:

$$E_1\, e_{11} = \sigma_{11} - \nu_{12}\, \sigma_{22} - \nu_{13}\, \sigma_{33} + E_1\, \alpha_1(T-T_o)$$

$$E_2\, e_{22} = -\nu_{21}\, \sigma_{11} + \sigma_{22} - \nu_{23}\, \sigma_{33} + E_2\, \alpha_2(T-T_o)$$

$$E_3\, e_{33} = -\nu_{31}\, \sigma_{11} - \nu_{32}\, \sigma_{22} + \sigma_{33} + E_3\, \alpha_3(T-T_o)$$

$$e_{12} = \frac{\sigma_{12}}{2\mu_{12}}$$

$$e_{13} = \frac{\sigma_{13}}{2\mu_{13}}$$

$$e_{23} = \frac{\sigma_{23}}{2\mu_{23}}. \qquad \text{(II 4)}$$

The E_i and ν_{ij} are Young's moduli and Poisson's ratios, the μ_{ij} are shear moduli, and the α_i are coefficients of thermal expansion. By regarding the $c_{ijk\ell}$ as coefficients obtained from solving (II 4) for the stresses, one finds

$$c_{1111} = E_1(1-\nu_{23}\nu_{32})/\Delta$$

$$c_{1122} = E_2(\nu_{12}+\nu_{13}\nu_{32})/\Delta = E_1(\nu_{21}+\nu_{31}\nu_{23})/\Delta$$

$$c_{1133} = E_3(\nu_{13}+\nu_{12}\nu_{23})/\Delta = E_1(\nu_{31}+\nu_{21}\nu_{32})/\Delta$$

$$c_{2222} = E_2(1-\nu_{13}\nu_{31})/\Delta$$

$$c_{2233} = E_3(\nu_{23}+\nu_{21}\nu_{13})/\Delta = E_2(\nu_{32}+\nu_{12}\nu_{31})/\Delta$$

$$c_{3333} = E_3(1-\nu_{12}\nu_{21})/\Delta$$

$$c_{1212} = \mu_{12}$$

$$c_{2323} = \mu_{23}$$

$$c_{1313} = \mu_{13}$$

$$c_{11} = -\left\{E_1\ \alpha_1(1-\nu_{23}\nu_{32}) + E_2\ \alpha_2(\nu_{12}+\nu_{32}\nu_{13}) + E_3\ \alpha_3(\nu_{13}+\nu_{23}\nu_{12})\right\}/\Delta$$

$$c_{22} = -\left\{E_1\ \alpha_1(\nu_{21}+\nu_{31}\nu_{23}) + E_2\ \alpha_2(1-\nu_{13}\nu_{31}) + E_3\ \alpha_3(\nu_{23}+\nu_{21}\nu_{13})\right\}/\Delta$$

$$c_{33} = -\left\{E_1\ \alpha_1(\nu_{31}+\nu_{21}\nu_{32}) + E_2\ \alpha_2(\nu_{32}+\nu_{31}\nu_{12}) + E_3\ \alpha_3(1-\nu_{12}\nu_{21})\right\}/\Delta$$

$$\Delta = 1 - \nu_{12}\nu_{21} - \nu_{13}\nu_{31} - \nu_{23}\nu_{32} - \nu_{12}\nu_{23}\nu_{31} - \nu_{21}\nu_{32}\nu_{13}. \qquad \text{(II 5)}$$

Symmetry of the coefficients in the equations for the stresses, (II 3), implies symmetry of the coefficients in (II 4) as follows:

$$\nu_{12} E_2 = \nu_{21} E_1, \nu_{13} E_3 = \nu_{31} E_1, \nu_{23} E_3 = \nu_{32} E_2,$$

$$\nu_{12}\nu_{23}\nu_{31} = \nu_{21}\nu_{32}\nu_{13}. \qquad \text{(II 6)}$$

Since the properties of the differential and difference equations for the displacement components, (I 11), are governed in part by the magnitudes of the elastic coefficients, it is important to find additional information about these coefficients. The requirement of stable thermodynamic equilibrium in terms of the free energy provides the needed facts. For the free energy given by (II 2) the requirement of stability is met if the quadratic part of F is positive definite.[2] Necessary and sufficient conditions for positive definiteness of the quadratic form are the positiveness of the principal minor determinants of the 6 x 6 matrix associated with the form. These conditions for the $c_{ijk\ell}$ are

(a) $c_{1111}, c_{2222}, c_{3333}, c_{1212}, c_{1313}, c_{2323} > 0,$

(b) $c_{1111}\, c_{2222} - c_{1122}^2 > 0,$

$c_{1111}\, c_{3333} - c_{1133}^2 > 0,$

$c_{2222}\, c_{3333} - c_{2233}^2 > 0,$

(c) $c_{1111}\, c_{2222}\, c_{3333} + 2c_{1122}\, c_{2233}\, c_{1133} - c_{1111}\, c^2_{2233}$

$$- c_{2232}\, c^2_{1133} - c_{3333}\, c^2_{1122} > 0. \qquad \text{(II 7)}$$

The three inequalities in (b) are symmetric forms equivalent to $\Delta > 0$, and (c) is independent of (a) and (b). The inverted form of the stress-strain relations (II 4) must also have a positive definite matrix and yields the inequalities

$$E_1,\ E_2,\ E_3,\ \mu_{12},\ \mu_{13},\ \mu_{23} > 0,$$

$$1 - \nu_{12}\,\nu_{21},\ 1 - \nu_{23}\,\nu_{32},\ 1 - \nu_{13}\,\nu_{31} > 0,$$

$$\Delta > 0. \qquad \text{(II 8)}$$

A necessary condition of positive definiteness is that the sum of the coefficients of the matrix be positive. Application of this condition to the first three equations of (II 4) with $T = T_o$ implies that the bulk modulus, k, defined by

$$\frac{1}{k} = \frac{e_{kk}}{-p} = \frac{1}{E_1} + \frac{1}{E_2} + \frac{1}{E_3} - \frac{\nu_{12}}{E_1} - \frac{\nu_{13}}{E_1} - \frac{\nu_{21}}{E_2} - \frac{\nu_{23}}{E_2} - \frac{\nu_{31}}{E_3} - \frac{\nu_{32}}{E_3} > 0 \qquad \text{(II 9)}$$

be positive and therefore

$$E_1\, E_2(1-\nu_{31}-\nu_{32}) + E_1\, E_3(1-\nu_{21}-\nu_{23}) + E_2\, E_3(1-\nu_{12}-\nu_{13}) > 0. \qquad \text{(II 10)}$$

Applied to the second order principal minors, the same arguments give

$$E_i + E_j \pm \nu_{ij} E_j \pm \nu_{ji} E_i > 0 \quad (i, j \text{ not summed}). \tag{II 11}$$

Inequalities (II 11) in conjunction with the symmetry conditions (II 6) give inequalities for the individual Poisson's ratios in terms of the Young's moduli,

$$\frac{E_i+E_j}{2E_i} > |\nu_{ij}|. \tag{II 12}$$

From (II 6) it should be noted that ν_{ij} and ν_{ji} always have the same sign.

If the orthotropic elastic constants of a particular material in terms of the $c_{ijk\ell}$ or E_i, μ_{ij}, ν_{ij} satisfy the inequalities (II 7) or (II 8), it can be concluded that the material tensor is positive definite. If the constants do not satisfy the inequalities, the constants are thermodynamically inconsistent and may not have been determined correctly by experiment, or the model which assumes the free energy to have the form (II 2) may not be physically adequate. In the latter case the material cannot be orthotropic, and a new form of the free energy must be found.

As is well known, positive definiteness of the free energy is also sufficient for the uniqueness within a rigid body motion to the boundary value problems of elasticity.[3]

The differential equations (I 11), for the displacement components in an orthotropic material can be written explicitly

$$(c_{1111} u_{1,1})_{,1} + (c_{1212} u_{1,2})_{,2} + (c_{1313} u_{1,3})_{,3}$$
$$+ (c_{1122} u_{2,2})_{,1} + (c_{1212} u_{2,1})_{,2}$$
$$+ (c_{1133} u_{3,3})_{,1} + (c_{1313} u_{3,1})_{,3} + (c_{11}[T-T_o])_{,1} = 0,$$

$$(c_{1212} u_{1,2})_{,1} + (c_{1122} u_{1,1})_{,2}$$
$$+ (c_{1212} u_{2,1})_{,1} + (c_{2222} u_{2,2})_{,2} + (c_{2323} u_{2,3})_{,3}$$
$$+ (c_{2233} u_{3,3})_{,2} + (c_{2323} u_{3,2})_{,3} + (c_{22}[T-T_o])_{,2} = 0,$$

$$(c_{1313} u_{1,3})_{,1} + (c_{1133} u_{1,1})_{,3}$$
$$+ (c_{2323} u_{2,3})_{,2} + (c_{2233} u_{2,2})_{,3}$$
$$+ (c_{1313} u_{3,1})_{,1} + (c_{2323} u_{3,2})_{,2} + (c_{3333} u_{3,3})_{,3}$$
$$+ (c_{33}[T-T_o])_{,3} = 0. \qquad \text{(II 13)}$$

If Equations (II 13) are written in the general form (I 11), the terms containing the highest derivatives are

$$c_{ijk\ell}\, u_{k,\ell j}. \qquad \text{(II 14)}$$

Since the quadratic form associated with the coefficient matrices is the free energy, which is assumed positive definite with respect to the strains, and if rigid motions are excluded, the form is also positive definite with respect to gradients of the displacement components. The differential equations associated with this form are therefore elliptic.[4]

In the case of plane strain, which will be investigated in detail, the strains satisfy

$$e_{i3} = 0. \tag{II 15}$$

The stress-strain relations for an orthotropic material reduce to

$$\sigma_{11} = c_{1111}\, u_{1,1} + c_{1122}\, u_{2,2} + c_{11}(T-T_o),$$

$$\sigma_{22} = c_{1122}\, u_{1,1} + c_{2222}\, u_{2,2} + c_{22}(T-T_o),$$

$$\sigma_{12} = c_{1212}(u_{1,2}+u_{2,1}). \tag{II 16}$$

The equilibrium equations in terms of displacements are

$$(c_{1111}\, u_{1,1})_{,1} + (c_{1212}\, u_{1,2})_{,2}$$

$$+ (c_{1212}\, u_{2,1})_{,2} + (c_{1122}\, u_{2,2})_{,1} + [c_{11}(T-T_o)]_{,1} = 0,$$

$$(c_{1212}\, u_{1,2})_{,1} + (c_{1122}\, u_{1,1})_{,2}$$

$$+ (c_{1212}\, u_{2,1})_{,1} + (c_{2222}\, u_{2,2})_{,2} + [c_{22}(T-T_o)]_{,2} = 0. \qquad \text{(II 17)}$$

The Helmholtz free energy is for plane strain

$$F = \frac{1}{2}(c_{1111}\, e_{11}^2 + c_{2222}\, e_{22}^2 + 2c_{1122}\, e_{11}\, e_{22} + 4c_{1212}\, e_{12}^2)$$

$$+ c_{11}\, e_{11}(T-T_o) + c_{22}\, e_{22}(T-T_o) + F(T_o) \qquad \text{(II 18)}$$

In the next section the free energy (II 18) will be used to obtain difference equations which approximate the differential equations (II 17) and the boundary conditions (I 8), (I 12), (I 13), and (I 14), appropriately modified for the plane case.

III. THE DIFFERENCE EQUATIONS FOR PLANE PROBLEMS

The difference equations for the plane problems will be derived from a variational principle equivalent to (I 3). In addition to the advantage of giving a positive semi-definite matrix, this approach offers a uniform method for forming the equations for the boundary points. For the current IBM 7090 code the boundary of the plane region is approximated by straight segments consisting of grid lines as shown in Figure 1. Future codes will approximate the boundaries by straight lines which are not necessarily grid lines. Difference equations for both boundary treatments will be presented although the current scheme will be examined in more detail. As before the coordinate surfaces are taken to be parallel to the planes of symmetry in the orthotropic material.

Using Greek indices to signify integers 1 or 2, we can write the variational principle as

$$\delta\iint_R \left[\frac{1}{2}c_{\alpha\beta\gamma\delta}\, u_{\alpha,\beta}u_{\gamma,\delta} + c_{\alpha\beta}\, u_{\alpha,\beta}(T-T_o)\right]dA - \delta\int_S T_\alpha u_\alpha dS = 0, \qquad \text{(III 1)}$$

where the first integral is over the entire plane region and the second is over that part of the boundary curve on which the stress vector is specified. The coefficients of the material appearing in (III 1) are those in (II 16) and (II 18). The variation, as before, is made on the displacements at constant temperature.

To obtain difference equations from (III 1) it suffices to approximate the integrals by sums and to approximate the derivatives in the integrand by differences. Application of the necessary conditions for a stationary value of the sum with respect to the displacement components yields the difference equations.

For the first scheme in which only square mesh cells appear, the free energy of a single cell with corner points denoted by (i,j), (i+1,j), (i+1,j+1), and (i,j+1) is a basic quantity. With material properties evaluated at the point (i,j) and with the derivatives at (i,j) obtained from fitting u_α by a plane through (i,j), (i+1,j), and (i,j+1), the energy in the cell with sides of length h is approximated by

$$\begin{aligned}\Bigg\{\frac{1}{2}\Bigg[& c_{1111ij}\left(\frac{u_{1i+1j}-u_{1ij}}{h^2}\right)^2 + 2c_{1122ij}\left(\frac{u_{1i+1j}-u_{1ij}}{h}\right)\left(\frac{u_{2ij+1}-u_{2ij}}{h}\right) \\ & + c_{2222ij}\left(\frac{u_{2ij+1}-u_{2ij}}{h^2}\right)^2 \\ & + 4c_{1212ij}\left(\frac{u_{1ij+1}-u_{1ij}}{2h} + \frac{u_{2i+1j}-u_{2ij}}{2h}\right)^2\Bigg] \\ & + c_{11ij}\left(\frac{u_{1i+1j}-u_{1ij}}{h}\right)(T-T_o)_{ij} + c_{22ij}\left(\frac{u_{2ij+1}-u_{2ij}}{h}\right)(T-T_o)_{ij}\Bigg\}h^2. \quad \text{(III 2)}\end{aligned}$$

Because the material tensor is positive definite with respect to the strains, (III 2) is semi-definite with respect to the displacement components. The energy in this cell could as well have been approximated by quadratic forms evaluated at the other corners (i+1,j), (i+1,j+1), and (i,j+1). A symmetric and still positive semi-definite form is obtained by averaging these four contributions to give the energy centered at $(i+\frac{1}{2},j+\frac{1}{2})$

$$
\begin{aligned}
q_{i+\frac{1}{2}\ j+\frac{1}{2}} = \tfrac{1}{2}\Big[& c_{1111ij}(u_{1i+1j}-u_{1ij})^2 + 2c_{1122ij}(u_{1i+1j}-u_{1ij})(u_{2ij+1}-u_{2ij}) \\
& + c_{2222ij}(u_{2ij+1}-u_{2ij})^2 + c_{1111i+1j}(u_{1i+1j}-u_{1ij})^2 \\
& + 2c_{1122i+1j}(u_{1i+1j}-u_{1ij})(u_{2i+1j+1}-u_{2i+1j}) \\
& + c_{2222i+1j}(u_{2i+1j+1}-u_{2i+1j})^2 + c_{1111i+1j+1}(u_{1i+1j+1}-u_{1i+1})^2 \\
& + 2c_{1122i+1j+1}(u_{1i+1j+1}-u_{1ij+1})(u_{2i+1j+1}-u_{2i+1j}) \\
& + c_{2222i+1j+1}(u_{2i+1j+1}-u_{2i+1j})^2 + c_{1111ij+1}(u_{1i+1j+1}-u_{1ij+1})^2 \\
& + 2c_{1122ij+1}(u_{1i+1j+1}-u_{1ij+1})(u_{2ij+1}-u_{2ij}) \\
& + c_{2222ij+1}(u_{2ij+1}-u_{2ij})^2 + c_{1212ij}(u_{1ij+1}-u_{1ij}+u_{2i+1j}-u_{2ij})^2
\end{aligned}
$$

$$+ c_{1212i+1j}(u_{1i+1j+1}-u_{1i+1j}+u_{2i+1j}-u_{2ij})^2$$

$$+ c_{1212i+1j+1}(u_{1i+1j+1}-u_{1i+1j}+u_{2i+1j+1}-u_{2ij+1})^2$$

$$+ c_{1212ij+1}(u_{1ij+1}-u_{1ij}+u_{2i+1j+1}-u_{2ij+1})^2\Big]$$

$$+ h[c_{11ij}(u_{1i+1j}-u_{1ij}) + c_{22ij}(u_{2ij+1}-u_{2ij})](T-T_o)_{ij}$$

$$+ h[c_{11i+1j}(u_{1i+1j}-u_{1ij}) + c_{22i+1j}(u_{2i+1j+1}-u_{2i+1j})](T-T_o)_{i+1j}$$

$$+ h[c_{11i+1j+1}(u_{1i+1j+1}-u_{1ij+1}) + c_{22i+1j+1}(u_{2i+1j+1}-u_{2i+1j})](T-T_o)_{i+1j+1}$$

$$+ h[c_{11ij+1}(u_{1i+1j+1}-u_{1ij+1}) + c_{22ij+1}(u_{2ij+1}-u_{2ij})](T-T_o)_{ij+1}. \quad \text{(III 3)}$$

The difference equations apart from the prescribed boundary terms are in every case obtained by minimizing a sum of cell energies like $q_{i+\frac{1}{2}\ j+\frac{1}{2}}$. It is convenient, therefore, to obtain the partial derivatives of $q_{i+\frac{1}{2}\ j+\frac{1}{2}}$ with respect to u_{1ij} and u_{2ij}. An interior point (ij) has neighboring cells with energies $q_{i+\frac{1}{2}\ j+\frac{1}{2}}$, $q_{i-\frac{1}{2}\ j+\frac{1}{2}}$, $q_{i-\frac{1}{2}\ j-\frac{1}{2}}$, and $q_{i+\frac{1}{2}\ j-\frac{1}{2}}$. Taking partial derivatives with respect to $u_{\alpha ij}$ of these four energies, we have eight basic quantities from which difference equations can be formed in a systematic way. The eight partial derivatives are

$$\frac{\partial q_{i+\frac{1}{2}j+\frac{1}{2}}}{\partial u_{1ij}} = -c_{1111ij}(u_{1i+1j}-u_{1ij}) - c_{1122ij}(u_{2ij+1}-u_{2ij})$$

$$-c_{1111i+1j}(u_{1i+1j}-u_{1ij}) - c_{1122i+1j}(u_{2i+1j+1}-u_{2i+1j})$$

$$-c_{1212ij}(u_{1ij+1}-u_{1ij}+u_{2i+1j}-u_{2ij})$$

$$-c_{1212ij+1}(u_{1ij+1}-u_{1ij}+u_{2i+ij+1}-u_{2ij+1})$$

$$-hc_{11ij}(T-T_o)_{ij} - hc_{11i+1j}(T-T_o)_{i+1j} ,$$

$$\frac{\partial q_{i+\frac{1}{2}j+\frac{1}{2}}}{\partial u_{2ij}} = -c_{1122ij}(u_{1i+1j}-u_{1i}) - c_{2222ij}(u_{2ij+1}-u_{2ij})$$

$$-c_{1122ij+1}(u_{1i+1j+1}-u_{1ij+1}) - c_{2222ij+1}(u_{2ij+1}-u_{2ij})$$

$$-c_{1212ij}(u_{1ij+1}-u_{1ij}+u_{2i+1j}-u_{2ij})$$

$$-c_{1212i+1j}(u_{1i+1j+1}-u_{1i+1j}+u_{2i+1j}-u_{2ij})$$

$$-hc_{22ij}(T-T_o)_{ij} - hc_{22ij+1}(T-T_o)_{ij+1} ,$$

$$\frac{\partial q_{i-\frac{1}{2}j+\frac{1}{2}}}{\partial u_{1ij}} = c_{1111ij}(u_{1ij}-u_{1i-1j}) + c_{1111i-1j}(u_{1ij}-u_{1i-1j})$$

$$+c_{1122ij}(u_{2ij+1}-u_{2ij}) + c_{1122i-1j}(u_{2i-1j+1}-u_{2i-1j})$$

$$-c_{1212ij}(u_{1ij+1}-u_{1ij}+u_{2ij}-u_{2i-1j})$$

$$-c_{1212ij+1}(u_{1ij+1}-u_{1ij}+u_{2ij+1}-u_{2i-1j+1})$$

$$+hc_{11ij}(T-T_o)_{ij} + hc_{11i-1j}(T-T_o)_{i-1j} ,$$

$$\frac{\partial q_{i-\frac{1}{2}j+\frac{1}{2}}}{\partial u_{2ij}} = -c_{2222ij}(u_{2ij+1}-u_{2ij}) - c_{2222ij+1}(u_{2ij+1}-u_{2ij})$$

$$-c_{1122ij}(u_{1ij}-u_{1i+1j}) - c_{1122ij+1}(u_{1ij}-u_{1i-1j+1})$$

$$+c_{1212ij}(u_{1ij+1}-u_{1ij}+u_{2ij}-u_{2i-1j})$$

$$+c_{1212i-1j}(u_{1i-1j+1}-u_{1i-1j}+u_{2ij}-u_{2i-1j})$$

$$-hc_{22ij}(T-T_o)_{ij} - hc_{22ij+1}(T-T_o)_{ij+1},$$

$$\frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{1ij}} = c_{1111ij}(u_{1ij}-u_{1i-1j}) + c_{1111i-1j}(u_{1ij}-u_{1i-1j})$$

$$+c_{1122ij}(u_{2ij}-u_{2ij-1}) + c_{1122i-1j}(u_{2i-1j}-u_{2i-1j-1})$$

$$+c_{1212ij}(u_{1ij}-u_{1ij-1}+u_{2ij}-u_{2i-1j})$$

$$+c_{1212ij-1}(u_{1ij}-u_{1ij-1}+u_{2ij-1}-u_{2i-1j-1})$$

$$+hc_{11ij}(T-T_o)_{ij} + c_{11i-1j}(T-T_o)_{i-1j},$$

$$\frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{2ij}} = c_{2222ij}(u_{2ij}-u_{2ij-1}) + c_{2222ij-1}(u_{2ij}-u_{2ij-1})$$

$$+c_{1122ij}(u_{1ij}-u_{1i-1j}) + c_{1122ij-1}(u_{1ij-1}-u_{1i-1j-1})$$

$$+c_{1212ij}(u_{1ij}-u_{1ij-1}+u_{2ij}-u_{2i-1j})$$

$$+c_{1212i-1j}(u_{1i-1j}-u_{1i-1j-1}+u_{2ij}-u_{2i-1j})$$

$$+hc_{22ij}(T-T_o)_{ij} + hc_{22ij-1}(T-T_o)_{ij-1},$$

$$\frac{\partial q_{i+\frac{1}{2}j-\frac{1}{2}}}{\partial u_{1ij}} = -c_{1111ij}(u_{1i-1j}-u_{1ij}) - c_{1111i+1j}(u_{1i+1j}-u_{1ij})$$

$$-c_{1122ij}(u_{2ij}-u_{2ij-1}) - c_{1122i+1j}(u_{2i+1j}-u_{2i+1j-1})$$

$$+c_{1212ij}(u_{1ij}-u_{1ij-1}+u_{2i+1j}-u_{2ij})$$

$$+c_{1212ij-1}(u_{1ij}-u_{1ij-1}+u_{2i+1j-1}-u_{2ij-1})$$

$$-hc_{11ij}(T-T_o)_{ij} - hc_{11i+1j}(T-T_o)_{i+1j} ,$$

$$\frac{\partial q_{i+\frac{1}{2}j-\frac{1}{2}}}{\partial u_{2ij}} = c_{2222ij}(u_{2ij}-u_{2ij-1}) + c_{2222ij-1}(u_{2ij}-u_{2ij-1})$$

$$+c_{1122ij}(u_{1i+1j}-u_{1ij}) + c_{1122ij-1}(u_{1i+1j-1}-u_{1ij-1})$$

$$-c_{1212ij}(u_{1ij}-u_{1ij-1}+u_{2i+1j}-u_{2ij})$$

$$-c_{1212i+1j}(u_{1i+1j}-u_{1i+1j-1}+u_{2i+1j}-u_{2ij})$$

$$+hc_{22ij}(T-T_o)_{ij} + hc_{22ij-1}(T-T_o)_{ij-1} . \qquad \text{(III 4)}$$

If the total free energy, Q, of the system is written as the sum of all the individual cell energies,

$$Q = \sum_k \sum_\ell q_{k\ell}; \qquad \text{(III 5)}$$

the difference equations for the point (ij) are

$$\frac{\partial Q}{\partial u_{\alpha ij}} = 0 \qquad \text{(III 6)}$$

unless the point is on a line of symmetry. Since the only terms of Q that can contribute to the expressions (III 6) are the eight partial derivatives (III 4) of the energies in the four adjacent cells of an interior point, the general difference equations for an interior point (ij) are

$$\frac{\partial q_{i+\frac{1}{2}j+\frac{1}{2}}}{\partial u_{\alpha ij}} + \frac{\partial q_{i-\frac{1}{2}j+\frac{1}{2}}}{\partial u_{\alpha ij}} + \frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{\alpha ij}} + \frac{\partial q_{i+\frac{1}{2}j-\frac{1}{2}}}{\partial u_{\alpha ij}} = 0. \qquad \text{(III 7)}$$

To obtain natural boundary conditions (specified stress vector) it is only necessary to note which types of cell energy can contribute and form a sum similar to (III 7). For example, consider a vertical boundary with the material on the left. The only energies which contribute to the difference equations are $q_{i-\frac{1}{2}j+\frac{1}{2}}$ and $q_{i-\frac{1}{2}j-\frac{1}{2}}$. The difference equations are, therefore,

$$\frac{\partial q_{i-\frac{1}{2}j+\frac{1}{2}}}{\partial u_{\alpha ij}} + \frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{\alpha ij}} - \overline{T}_{\alpha} 2h = 0 \qquad \text{(III 8)}$$

where $\overline{T}_{\alpha}$ are averaged components of the specified stress vector on the boundary of the two cells.

For a corner point on the boundary the cell energy contributing might be $q_{i+\frac{1}{2}j-\frac{1}{2}}$. The difference equations would be

$$\frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{\alpha ij}} - \overline{T}_{\alpha} 2h = 0. \qquad \text{(III 9)}$$

All the other specified stress cases can be treated in a similar way.

The boundary conditions at an internal line of symmetry can be obtained by minimizing the energy with respect to the tangential displacement vector only. As the most simple example consider again a vertical symmetry boundary. For this case $u_{1ij} = 0$, and u_{2ij} is to be varied. The difference equation is simply

$$\frac{\partial q_{i-\frac{1}{2}j+\frac{1}{2}}}{\partial u_{2ij}} + \frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{2ij}} = 0 \qquad \text{(III 10)}$$

which with $u_{1ij} = 0$ form the boundary conditions.

For the more general situation where the symmetry line runs at an angle through the mesh, the u_1 and u_2 components are related by

$$u_n = u_1 n_1 + u_2 n_2 = 0. \qquad \text{(III 11)}$$

Variation of the energy in a cell must take this constraint into account. If u_1 is taken to be the independent variable, only the variation of the energy with respect to u_1 is taken. Consider again the case where the symmetry line is replaced by a segment of mesh lines and the cell whose energy contributes terms to the difference equation is centered at $i-\frac{1}{2}j-\frac{1}{2}$. The difference equation is then

$$\frac{dq_{i-\frac{1}{2}j-\frac{1}{2}}}{du_{1ij}} = \frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{1ij}} + \frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{2ij}}\left(-\frac{n_1}{n_2}\right) = 0. \qquad \text{(III 12)}$$

The tangent vector at the point ij which approximates a boundary point has components

$$t_1 = -n_2, \; t_2 = n_1. \qquad \text{(III 13)}$$

Equation (III 10) is therefore

$$\frac{\partial q_{i-\frac{1}{2}j-\frac{1}{2}}}{\partial u_{\alpha ij}} t_\alpha = 0. \qquad \text{(III 14)}$$

Thus (III 11) and (III 14) are the approximate boundary conditions for the case of a symmetry boundary not coincident with a mesh line. In view of Equation (III 9) it is evident that (III 14) is an approximation to the natural part of the symmetry boundary conditions (I 14) $T_t = \sigma_{\alpha\beta} n_\beta t_\alpha = 0$.

Comparison by a Taylor's expansion of the interior difference equations (III 7) with the differential equations (II 17) shows that the error is of order h^2. On the boundary lack of symmetry in the difference equations gives an error of order h. Part of the boundary error must be ascribed to the distorted boundary which is used when all mesh cells are required to be square. In order to reduce this latter error, a modification of the boundary treatment will now be presented.

The treatment proposed is based on an approximation of the boundary by chords between points of intersection of the boundary curve with mesh cells, Figure 2. In order to keep the number of possible configurations to a minimum it will be assumed that the mesh size is so small that the boundary curve does not pass through the sides of any cell more than twice. That part of a boundary cell which belongs to the interior is then a triangle, a quadrilateral, or a pentagon.

The quantity needed for the difference equations of points on or adjacent to the boundary is the free energy associated with such irregular shaped areas. The energy in a square cell was calculated by averaging an energy associated with each of the four vertices. If each of the four vertices is assumed to account for the energy in a triangle consisting of the vertex in question and its two neighbors, then the sum of the energy of all four possible such triangles is twice that of the whole cell. The sum of the triangular energies is therefore divided by two. A similar approach is to be used for the irregular regions.

The derivates of the displacements needed for the energy in a triangular region can be obtained by passing a plane representing u_α through the three vertices of the triangle. The displacements in the plane can be represented by an expression of the term

$$u_\alpha = a^{ij}_{\alpha\gamma} x_\gamma + b_\alpha \qquad \text{(III 15)}$$

where i and j are indices locating what might be called the primary vertex, and where (i+1j), (ij+1) are the other vertices. The derivative of u_α at the point (ij) is

$$u^{ij}_{\alpha,\beta} = a^{ij}_{\alpha\beta}, \tag{III 16}$$

and the energy associated with this triangle becomes

$$\begin{aligned} q^{T}_{ij} = \Big\{ \tfrac{1}{2} \Big[& c_{1111ij}(a^{ij}_{11})^2 + 2c_{1122ij}\, a^{ij}_{11}\, a^{ij}_{22} + c_{2222ij}(a^{ij}_{22})^2 \\ & + 4c_{1212ij}(a^{ij}_{12}+a^{ij}_{21})^2 \Big] \\ & + c_{11ij}\, a^{ij}_{11}(T-T_o)_{ij} + c_{11ij}\, a^{ij}_{22}(T-T_o)_{ij} \Big\} A_{ij}, \end{aligned} \tag{III 17}$$

where A_{ij} is the area of the triangle. Since there are three vertices to the triangle, a more symmetric form of the energy is

$$q^{T}_{i+\frac{1}{2}j+\frac{1}{2}} = \frac{q^{T}_{ij} + q^{T}_{i+1j} + q^{T}_{ij+1}}{3}. \tag{III 18}$$

For a quadrilateral the treatment is the same as that for a square, the energies of the four triangles formed by passing diagonals through the vertices are averaged,

$$q^{Q} = \frac{q^{T}_{ij} + q^{T}_{i+1j} + q^{T}_{ij+1} + q^{T}_{i+1j+1}}{2}. \tag{III 19}$$

The pentagonal boundary region presents a larger number of possible subdivisions for computing the energy from its component triangles. From the coding viewpoint the simplest expedient would be to readjust the approximate boundary so that all pentagons are altered into quadrilaterals. Next in order of complexity would be a somewhat arbitrary division of the pentagon into a quadrilateral and a triangle. A third possibility, having less bias, would be to obtain three triangles associated with each of the five vertices by passing lines from the given vertex to all the others. Fifteen triangular energies would be computed in this way whose sum was five times the energy of the pentagon. If the vertices were labelled as in Figure 3, and the energies associated with vertex one written q_{123}, q_{134}, q_{145}, the total energy of the cell becomes

$$q^P = 1/5\Big[2q^T_{123} + q^T_{134} + 2q^T_{145} + q^T_{245} + 2q^T_{145} + q^T_{315} + 2q^T_{234} + q^T_{412} + 2q^T_{345} + q^T_{523}\Big]. \qquad \text{(III 20)}$$

To obtain the difference equations for regions made of triangles one forms sums of terms like

$$\frac{\partial q^T_{i+\frac{1}{2}j+\frac{1}{2}}}{\partial u_{\alpha ij}} = 0. \qquad \text{(III 21)}$$

This equation in turn is formed from the derivatives of the energies in triangles according to (III 18). Thus the basic derivatives are

$$\frac{\partial q^T_{ij}}{\partial u_{\alpha ij}} = 0. \tag{III 22}$$

From elementary considerations the quantities $a_{\alpha\beta}$ appearing in the Equations (III 16) and (III 17) are

$$a^{ij}_{11} = \Big[u_{1i+1j}(x_{2ij+1}-x_{2ij}) - u_{2i+1j}(x_{2i+1j}-x_{2ij})$$
$$- u_{1ij}(x_{2ij+1}-x_{2i+1j})\Big]/2A_{ij} \ ,$$

$$a^{ij}_{22} = \Big[u_{2ij+1}(x_{1i+1j}-x_{1ij}) - u_{2i+1j}(x_{1ij+1}-x_{1ij})$$
$$- u_{2ij}(x_{1i+1j}-x_{1ij+1})\Big]/2A_{ij},$$

$$a^{ij}_{12} = \Big[u_{1ij+1}(x_{1i+1j}-x_{1ij}) - u_{1i+1j}(x_{1ij+1}-x_{1ij})$$
$$+ u_{1ij}(x_{1i+1j}-x_{1ij+1})\Big]/2A_{ij},$$

$$a^{ij}_{21} = \Big[u_{2ij+j}(x_{2ij+1}-x_{2ij}) - u_{2ij+1}(x_{2i+1j}-x_{2ij})$$
$$- u_{2ij}(x_{2ij+1}-x_{2i+1j})\Big]/2A_{ij}. \tag{III 23}$$

From (III 17),

$$\frac{\partial q^T_{ij}}{\partial u_{\alpha ij}} = \left[c_{1111ij}\, a^{ij}_{11} \frac{\partial a^{ij}_{11}}{\partial u_{\alpha ij}} + c_{1122ij}\left(\frac{\partial a^{ij}_{11}}{\partial u_{\alpha ij}}\, a^{ij}_{22} + a^{ij}_{11} \frac{\partial a^{ij}_{22}}{\partial u_{\alpha ij}}\right)\right.$$

$$+ c_{2222ij}\, a^{ij}_{22} \frac{\partial a^{ij}_{22}}{\partial u_{\alpha ij}}$$

$$+ 8c_{1212ij}\left(a^{ij}_{12} + a^{ij}_{21}\right)\left(\frac{\partial a^{ij}_{12}}{\partial u_{\alpha ij}} + \frac{\partial a^{ij}_{21}}{\partial u_{\alpha ij}}\right)$$

$$\left. + c_{11ij}(T-T_o)_{ij} \frac{\partial a^{ij}_{11}}{\partial u_{\alpha ij}} + c_{22ij}(T-T_o)_{ij} \frac{\partial a^{ij}_{22}}{\partial u_{\alpha ij}}\right] A_{ij}. \qquad \text{(III 24)}$$

But

$$\frac{\partial a^{ij}_{11}}{\partial u_{\alpha ij}} = -\frac{(x_{2ij+1} - x_{2i+1j})}{2A_{ij}}\, \delta_{\alpha 1},$$

$$\frac{\partial a^{ij}_{22}}{\partial u_{\alpha ij}} = -\frac{(x_{1i+1j} - x_{1ij+1})}{2A_{ij}}\, \delta_{\alpha 2},$$

$$\frac{\partial a^{ij}_{12}}{\partial u_{\alpha ij}} = -\frac{(x_{1i+1j} - x_{1ij+1})}{2A_{ij}}\, \delta_{\alpha 1},$$

$$\frac{\partial a^{ij}_{21}}{\partial u_{\alpha ij}} = -\frac{(x_{2ij+1} - x_{2i+1j})}{2A_{ij}}\, \delta_{\alpha 2}.$$

Thus

$$
\begin{aligned}
\frac{\partial q^T_{ij}}{\partial u_{\alpha ij}} = \Big\{ & c_{1111ij}[u_{1i+1j}(x_{2ij+1}-x_{2ij}) - u_{1ij+1}(x_{2i+1j}-x_{2ij}) \\
& - u_{1ij}(x_{2ij+1}-x_{2i+1j})][x_{2i+1j}-x_{2ij+1}]\delta_{\alpha 1} \\
& + c_{1122ij}[u_{1i+1j}(x_{2ij+1}-x_{2ij}) - u_{1ij+1}(x_{2i+1j}-x_{2ij}) \\
& - u_{1ij}(x_{2ij+1}-x_{2i+1j})][x_{1ij+1}-x_{1i+1j}]\,\delta_{\alpha 2} \\
& + c_{1122ij}[u_{2ij+1}(x_{1i+1j}-x_{1ij}) - u_{2i+1j}(x_{1ij+1}-x_{1ij}) \\
& - u_{2ij}(x_{1i+1j}-x_{1ij+1})][x_{2i+1j}-x_{2ij+1}]\,\delta_{\alpha 1} \\
& + c_{2222ij}[u_{2ij+1}(x_{1i+1j}-x_{1ij}) - u_{2i+1j}(x_{1ij+1}-x_{1ij}) \\
& - u_{2ij}(x_{1i+1j}-x_{2ij+1})][x_{1ij+1}-x_{1i+1j}]\,\delta_{\alpha 2} \\
& + 8c_{1212ij}[u_{1ij+1}(x_{1i+1j}-x_{1ij}) - u_{1i+1j}(x_{1ij+1}-x_{1ij}) \\
& - u_{1ij}(x_{1i+1j}-x_{1ij+1}) + u_{2i+1j}(x_{2ij+1}-x_{2ij}) \\
& - u_{2ij+1}(x_{2i+1j}-x_{2ij}) - u_{2ij}(x_{2ij+1}-x_{2i+1j})] \\
& \times[(x_{1ij+1}-x_{1i+1j})\delta_{\alpha 1} + (x_{2i+1j}-x_{2ij+1})\delta_{\alpha 2}] \\
& + c_{11ij}(T-T_o)_{ij}(x_{2i+1j}-x_{2ij+1})\delta_{\alpha 1} \\
& + c_{22ij}(T-T_o)_{ij}(x_{1ij+1}-x_{1i+1j})\delta_{\alpha 2}\Big\}/2A_{ij}\,,
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial q^T_{ij}}{\partial u_{\alpha ij}} = \Big\{ & [u_{1i+1j}(x_{2ij+1}-x_{2ij}) - u_{1ij+1}(x_{2i+1j}-x_{2ij}) \\
& - u_{1ij}(x_{2ij+1}-x_{2i+1j})][c_{1111ij}(x_{2i+1j}-x_{2ij+1})\delta_{\alpha 1} \\
& + c_{1122ij}(x_{1ij+1}-x_{1i+1j})\delta_{\alpha 2}] + [u_{2ij+1}(x_{1i+1j}-x_{1ij}) \\
& - u_{2i+1j}(x_{1ij+1}-x_{1ij}) - u_{2ij}(x_{1i+1j}-x_{2ij+1})] \\
& \times [c_{1122ij}(x_{2i+1j}-x_{2ij+1})\delta_{\alpha 1} + c_{2222ij}(x_{1ij+1}-x_{1i+1j})\delta_{\alpha 2}] \\
& + 8c_{1212ij}[u_{1ij+1}(x_{1i+1j}-x_{1ij}) - u_{1i+1j}(x_{1ij+1}-x_{1ij}) \\
& - u_{1ij}(x_{1i+1j}-x_{1ij+1}) + u_{2i+1j}(x_{2ij+1}-x_{2ij}) \\
& - u_{2ij+1}(x_{2i+1j}-x_{2ij}) - u_{2ij}(x_{2ij+1}-x_{2i+1j})] \\
& \times [(x_{1ij+1}-x_{i+1j})\delta_{\alpha 1} + (x_{2i+1j}-x_{2ij+1})\delta_{\alpha 2}] \\
& + c_{11ij}(T-T_o)_{ij}(x_{2i+1j}-x_{2ij+1})\delta_{\alpha 1} \\
& + c_{22ij}(T-T_o)_{ij}(x_{1ij+1}-x_{1i+1j})\delta_{\alpha 2}\Big\}/2A_{ij}. \qquad \text{(III 25)}
\end{aligned}
$$

Expressions for $\partial q^T_{i+1j}/\partial u_{\alpha ij}$ and $\partial q^T_{ij+1}/\partial u_{\alpha ij}$ can be obtained in a similar manner to form the complete derivative of the cell energy $\partial q^T_{i+\frac{1}{2}j+\frac{1}{2}}/\partial u_{\alpha ij}$. It is apparent at this time that the price paid for a more careful boundary treatment is not only a much greater complexity in the coefficients of the difference equations but also a proliferation of possible combinations of cell arrangements at the boundary with an attendant difficulty in the logic of coding any automatic routines for setting up the mesh and the difference equations.

IV. NUMERICAL CALCULATION OF THE STRESSES IN AN INFINITE HOLLOW CYLINDER

In order to test the difference equations of plane elasticity derived in Section III, the following example problem was considered. An infinite hollow cylinder of isotropic material was assumed to have a temperature distribution varying inversely with the radius. The inner surface was stress free; the outer was held fixed.

For the numerical calculation a section of the annulus between 0° and 60° was chosen for the region of integration. Thus there was one symmetry boundary coincident with the x-axis, and the other symmetry boundary was at 60°. Because the basic mesh cells for the difference equations are square, the displacement specified, 60° symmetry, and stress free boundaries were zig-zag. In Fig. (4A) the segment of the annulus and in Fig. (4B) its approximation by zig-zag and straight boundary sections are shown. The boundary for the numerical solution is identified by numbers 1 - 9 and letters A - U. The letter "O" identifies interior points, the letter "V" exterior points. The numbers and letters on the boundary tell the automatic set-up code which type of boundary condition (stress, displacement, or symmetry) is in effect and which of the cell energies are going to contribute to the difference equations for the point. Fig. (4) is a reproduction from film taken of a plot with a Benson-Lehner 4020.

The analytic solution to the hollow cylinder problem is in polar coordinates,

$$\frac{u_r}{a} = -\frac{(1+\nu)}{(1-\nu)}\,\alpha\,T_i\,\frac{a}{r}\left(\frac{b}{a}-1\right)\left[\frac{1+(1-2\nu)\left(\frac{r}{a}\right)^2}{1+(1-2\nu)\left(\frac{b}{a}\right)^2} - \frac{\left(\frac{r}{a}-1\right)}{\left(\frac{b}{a}-1\right)}\right],$$

$$\frac{\sigma_r}{E} = -\frac{\alpha T_i}{1-\nu}\left(1-\frac{a}{r}\right)\left[\frac{a}{r} + \frac{\left(\frac{b}{a}-1\right)}{1+(1-2\nu)\left(\frac{b}{a}\right)^2}\left(1+\frac{a}{r}\right)\right],$$

$$\frac{\sigma_\theta}{E} = -\frac{\alpha T_i}{1-\nu}\left[\frac{\left(\frac{b}{a}-1\right)}{1+(1-2\nu)\left(\frac{b}{a}\right)^2}\left[1+\left(\frac{a}{r}\right)^2\right] + \left(\frac{a}{r}\right)^2\right]. \qquad \text{(IV 1)}$$

In the above formulae a is the inner radius, b the outer, T_i the temperature at a. The isotropic elastic constants, E, ν, and α, have the usual significance. The cartesian components corresponding to (IV 1) are

$$u_1 = u_r \cos\theta,$$

$$u_2 = u_r \sin\theta,$$

$$\frac{\sigma_{11}}{E} = \frac{\sigma_r}{E}\cos^2\theta + \frac{\sigma_\theta}{E}\sin^2\theta,$$

$$\frac{\sigma_{12}}{E} = \sin\theta \cos\theta\left(\frac{\sigma_r}{E} - \frac{\sigma_\theta}{E}\right),$$

$$\frac{\sigma_{22}}{E} = \frac{\sigma_r}{E}\sin^2\theta + \frac{\sigma_\theta}{E}\cos^2\theta. \qquad \text{(IV 2)}$$

The components u_1 and u_2 of (IV 2) are to be compared with the displacements calculated from general difference equations (III 7) and the various boundary difference equations (III 8), (III 9), etc. The stresses of (IV 2) are to be compared with stresses obtained by differencing the numerical displacements to form approximate strains and by use of the stress-strain relations (II 16) with isotropic constants. The approximate strains, computed from displacements at the corners of square mesh cells, are centered at the centroid of each cell. The stresses obtained are therefore not to be compared with the boundary stresses of the analytic solution but with analytic stresses slightly removed from the boundary.

The numerical problem was solved for the following values of the parameters:

$$a = 5.0 \text{ cm},$$
$$b = 10.0 \text{ cm},$$
$$h = 0.25 \text{ cm},$$
$$T_i = 5000^\circ C,$$
$$\nu = 0.3,$$
$$\alpha = 8 \times 10^{-6}/^\circ C \qquad \text{(IV 3)}$$

The method used for solving the linear system of equations was successive over-relaxation with extrapolation.[5] No attempt was made to optimize the extrapolation parameter ω in this particular calculation, although the value of ω, equal to 1.6, was chosen on the basis of an earlier set of problems. The computer program consists of a mesher, which will set up the boundary and interior points and their difference equations, a relaxation code for the displacements with a check on residuals, and a stress calculator. All of these programs were written by L. Stein in Ivy, a compiler-assembler at LASL for the IBM 7040 and IBM 7090. The number of calculated mesh points was 691. Running time until the maximum residual was reduced to 10^{-8} was about 25 minutes or 750 cycles on the IBM 7090.

The results of the calculation of displacement are compared with the analytical radial displacement in Figures 5-7. The calculated stress is compared with the analytic stress on each of the four boundaries and in the interior on a radius of 45°. These are shown in Figures 8-22. While the displacement is sufficiently accurate on the boundary and in the interior, the stress is naturally less accurate, particularly on the boundary.

Considering the fact that the zig-zag boundary was assumed to satisfy the same boundary conditions that are correct for the true boundary, the loss of accuracy at the boundary was not unexpected. Smoothness of the stress and displacement in the interior suggested that values could be extrapolated to the zig-zag boundaries which could then be used to obtain an improved solution particularly near the boundary where the effect would be greatest. Adjustment of the displacement boundary conditions at the outer radius was performed with the improved results in the stress shown on part of that boundary in Figures 17-19. Adjustment of stress free boundary was tried at the worst point on the boundary with the results shown in Figures 11-13. To be really effective an extrapolation scheme of this type should be made part of the program for the computing machine. Also an investigation should be made to determine whether such an iteration of boundary values is an always convergent process.

Another procedure for handling difficult areas near the boundary is made feasible by the existence of L. Stein's meshing code. The subregion in which difficulty is encountered can be removed from the rest of the problem and its number of calculation points increased. Boundary values for the artificial boundary created can be obtained from a first run for the real region of integration. The automatic mesher makes such a refined calculation straightforward, whereas set-up by hand for a large number of points is tedious and time-consuming.

It might be thought that a differencing scheme for the boundary points based on interpolation to the correct boundary location would be an answer to the difficulties encountered on the boundary. Such an approach was taken in an early attempt on this problem, but the iteration process failed to converge. The total matrix of the difference equations was too complex to analyze, and that approach was abandoned for the variational derivation. An attempt to obtain interpolation formulae which would necessarily leave the matrix of total equations positive definite should be made. Still to be tried are the more complicated energy relations based on triangular regions described in the latter part of Section III.

It is hoped that further investigation of the techniques at the boundary will yield a practicable and simple solution to the problem of accuracy at the boundary which is an inherent difficulty with elliptic equations. In the meantime the present scheme based on square cells should provide displacements of sufficient accuracy and, with the adjustment of boundary values and boundary mesh refinement, stresses of useful accuracy as well.

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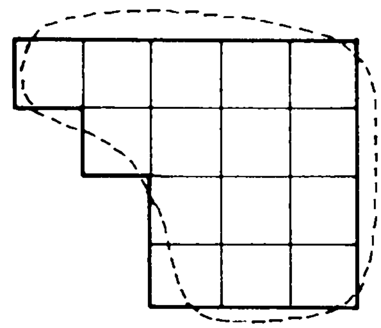
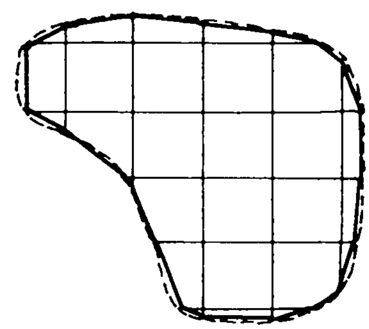
Figure 1



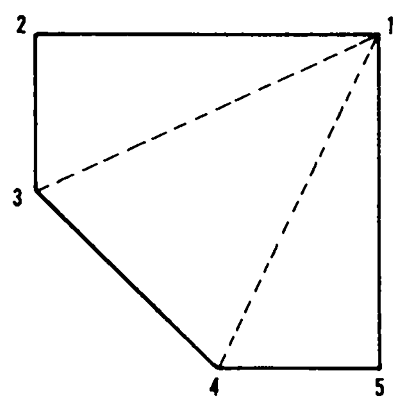
Approximation of boundary by grid lines.

Figure 2



Approximation of boundary by chords.

Figure 3



Pentagonal boundary cell.

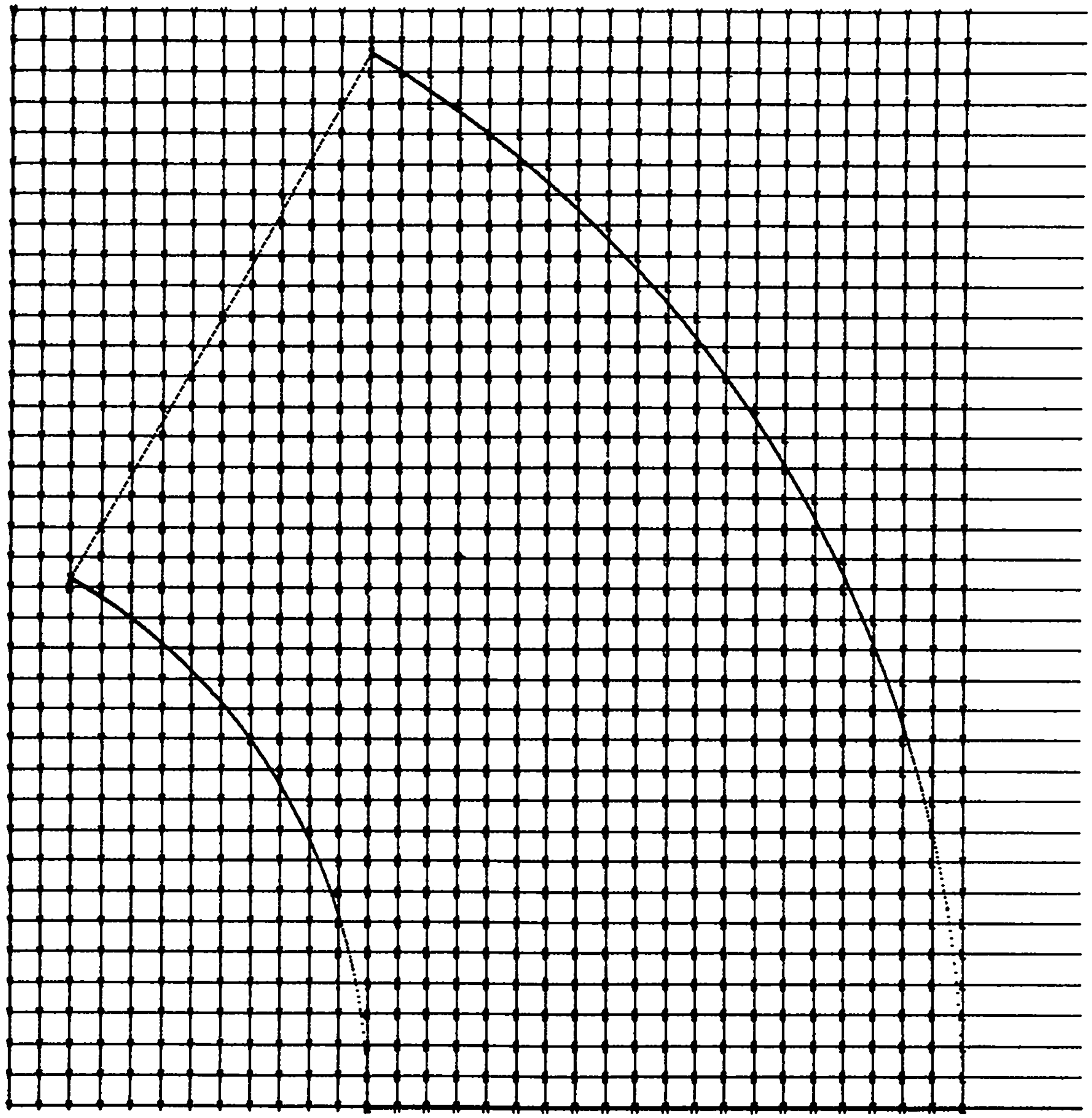


Figure 4A. Print of annular section

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V V V V V V V V V V V V V V V V V V V V V V V V V V V V V V V V V
V V V V V V V V V V V V V V V V V V V V V V V V V V V V V V V V V
V V V V V V V V V V V G L L L V V V V V V V V V V V V V V V V V V
V V V V V V V V V V V K 0 0 L L V V V V V V V V V V V V V V V V V
V V V V V V V V V V G P 0 0 0 L L L V V V V V V V V V V V V V V V
V V V V V V V V V V K 0 0 0 0 0 0 L L V V V V V V V V V V V V V V
V V V V V V V V V G P 0 0 0 0 0 0 0 L L V V V V V V V V V V V V V
V V V V V V V V G P 0 0 0 0 0 0 0 0 0 L L V V V V V V V V V V V V
V V V V V V V V K 0 0 0 0 0 0 0 0 0 0 0 L L V V V V V V V V V V V
V V V V V V V G P 0 0 0 0 0 0 0 0 0 0 0 0 L L V V V V V V V V V V
V V V V V V V K 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L L V V V V V V V V V
V V V V V V G P 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L L V V V V V V V V
V V V V V V K 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L V V V V V V V V
V V V V V G P 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L L V V V V V V V
V V V V G P 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L L V V V V V V
V V V V K 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L V V V V V V
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V V D 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L V V V V
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V V V V V V V V V V 8 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L V
V V V V V V V V V V 1 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L V
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V V V V V V V V V V V 8 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L
V V V V V V V V V V V 1 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L
V V V V V V V V V V V V 8 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 L
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Figure 4B. Print of mesh point identification

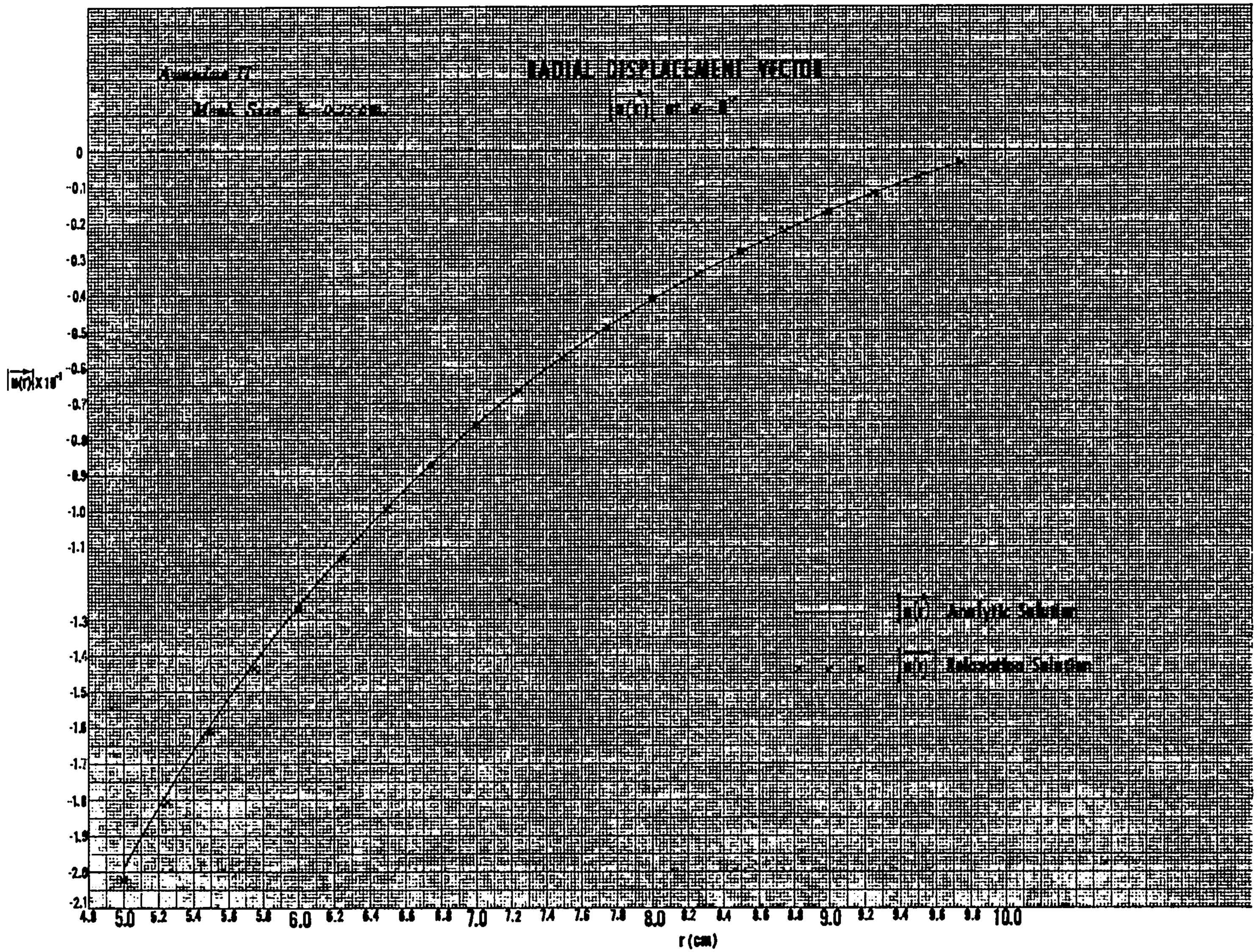

Figure 5. Radial displacement, $\Theta = 0^{\circ}$

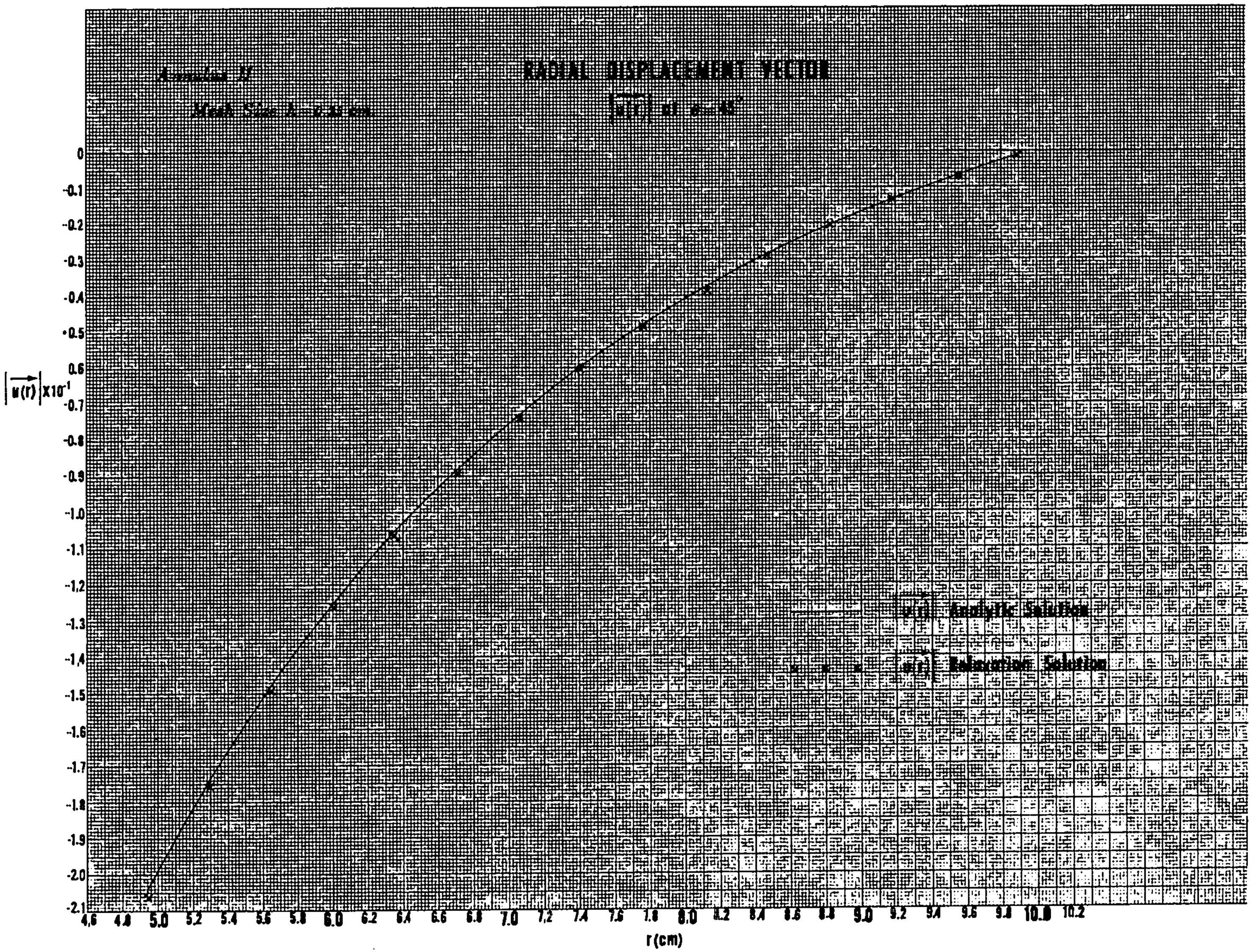

Figure 6. Radial displacement, $\Theta = 45^{\circ}$

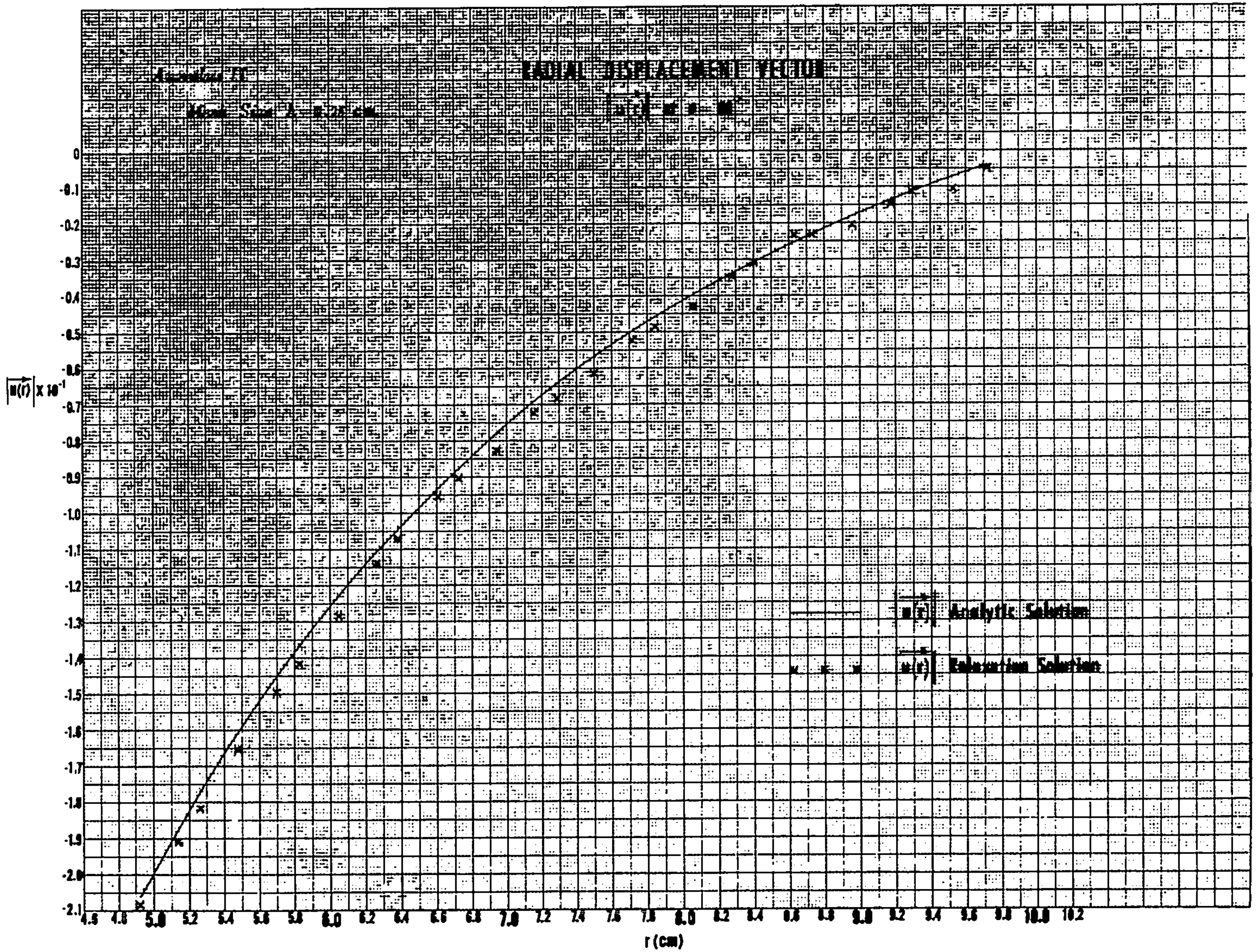

Figure 7. Radial displacement, $\Theta = 60^{\circ}$

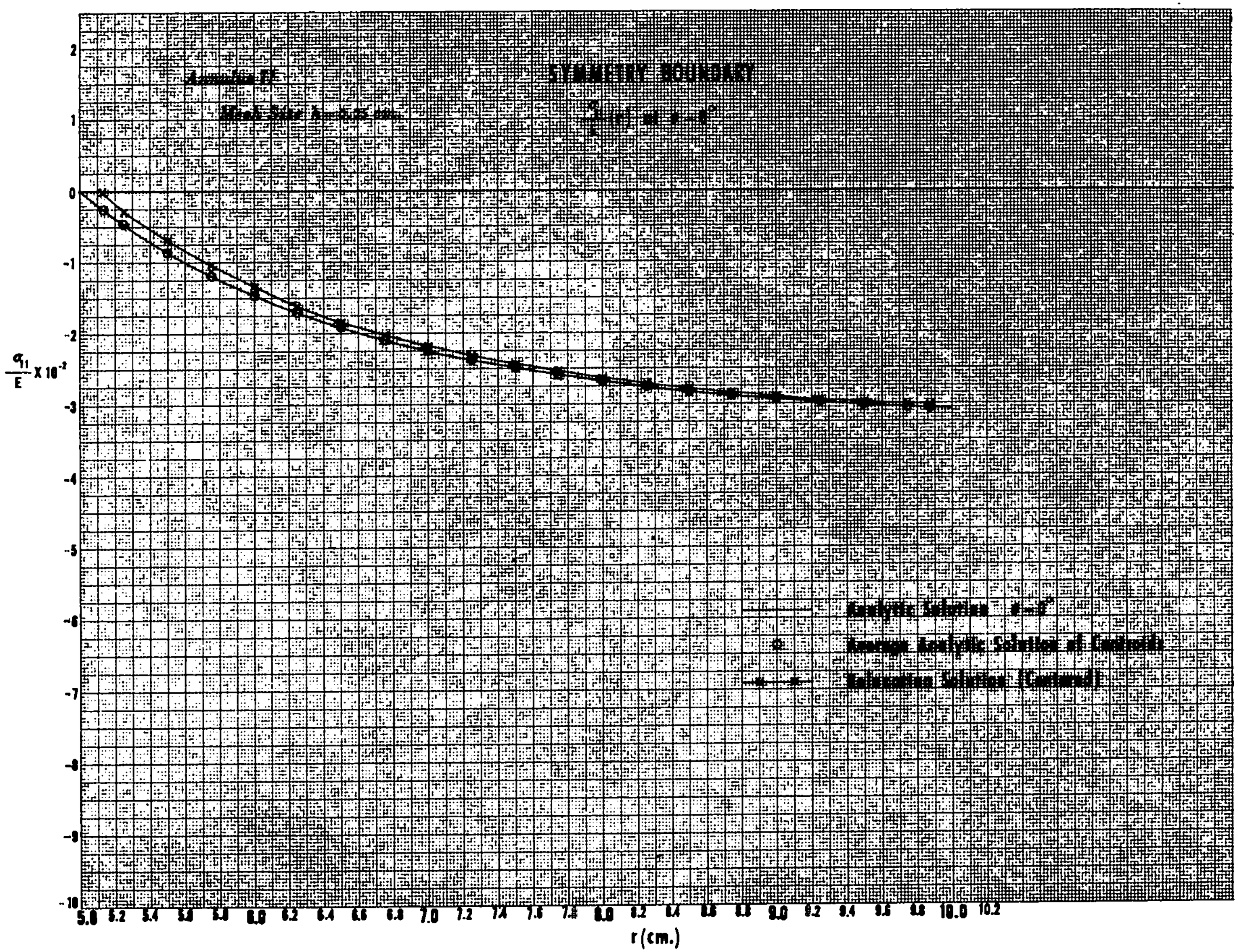

Figure 8. σ_{11} symmetry boundary, $\Theta = 0^{\circ}$

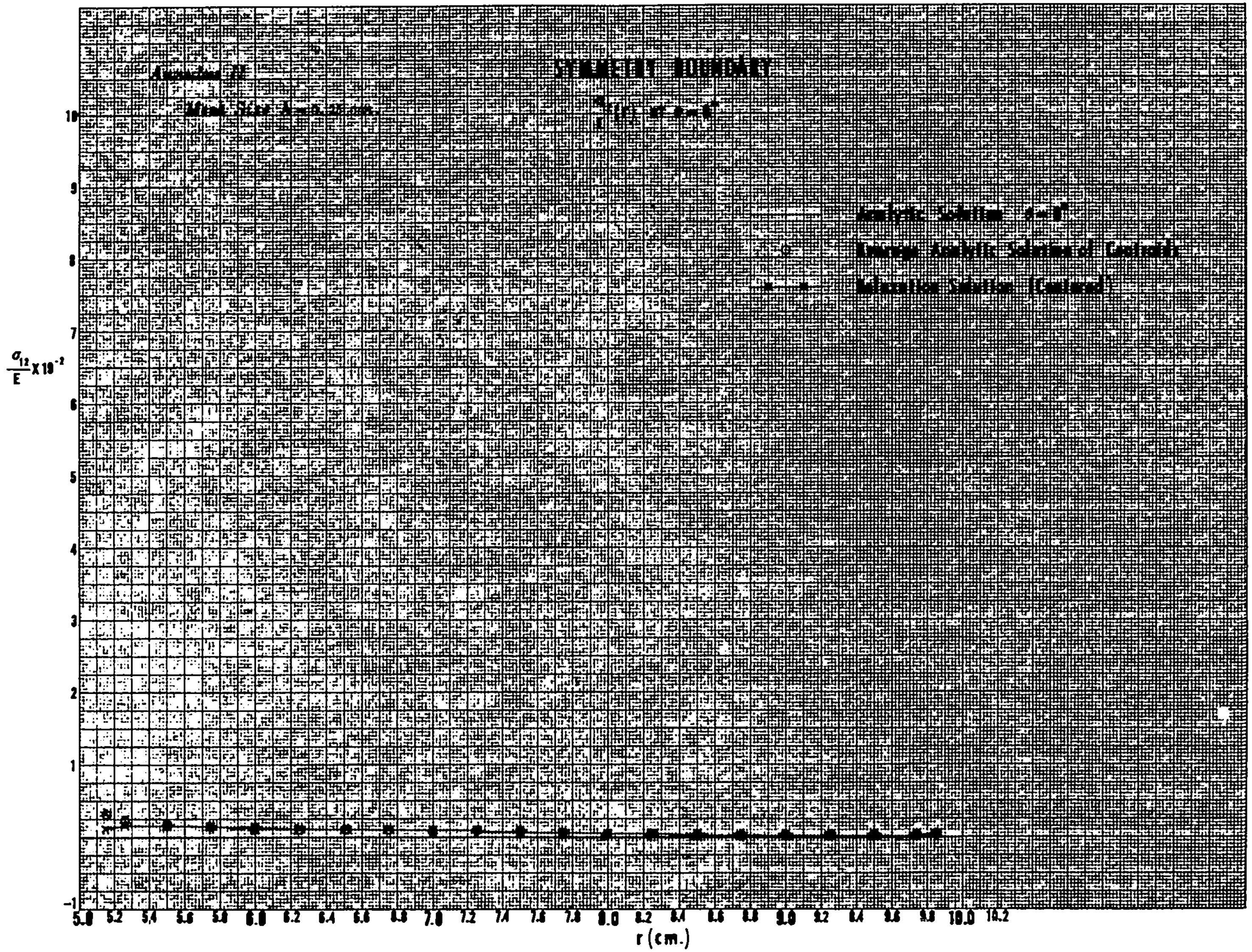

Figure 9. σ_{12} symmetry boundary, $\Theta = 0^{\circ}$

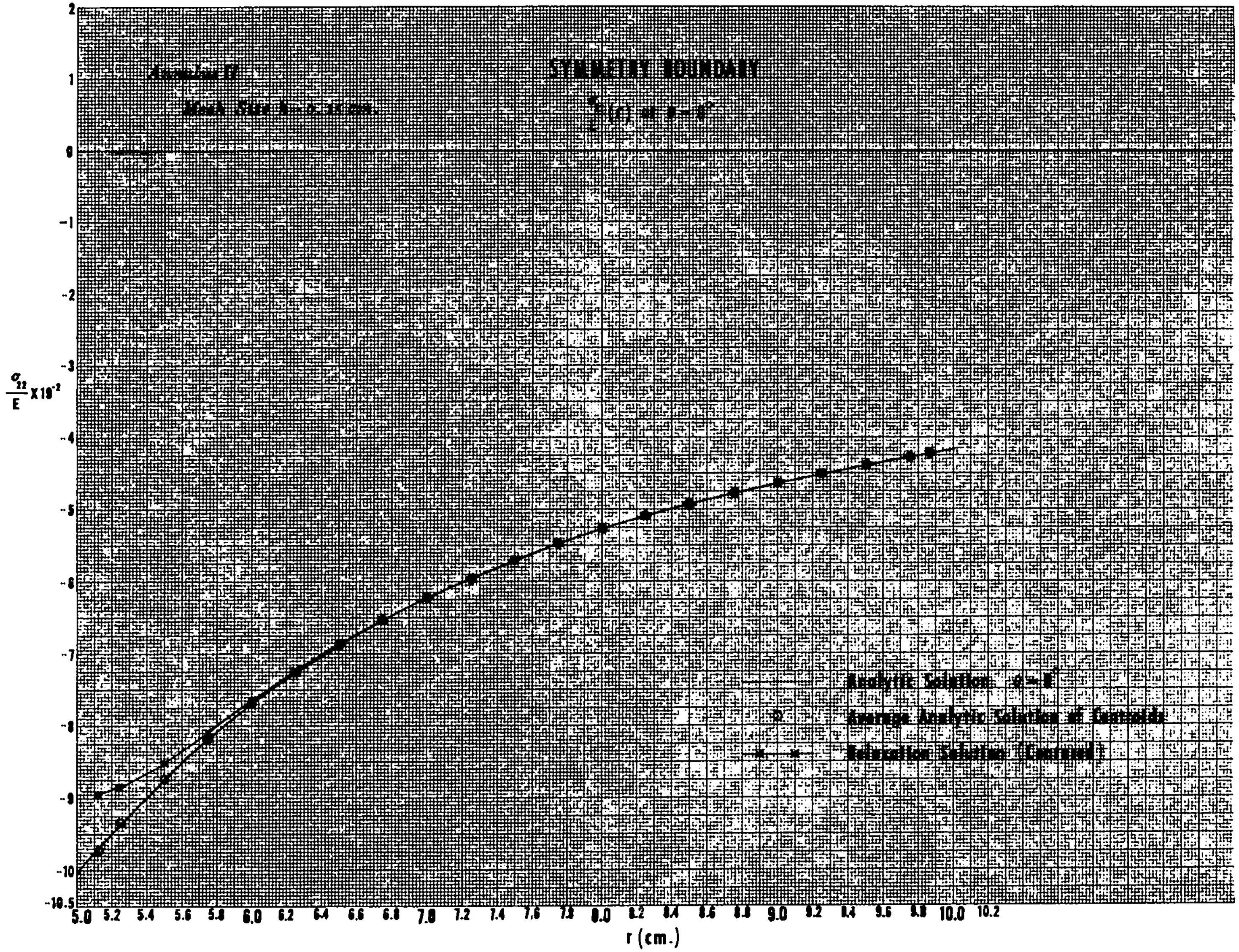

Figure 10. σ_{22} symmetry boundary, $\Theta = 0^{\circ}$

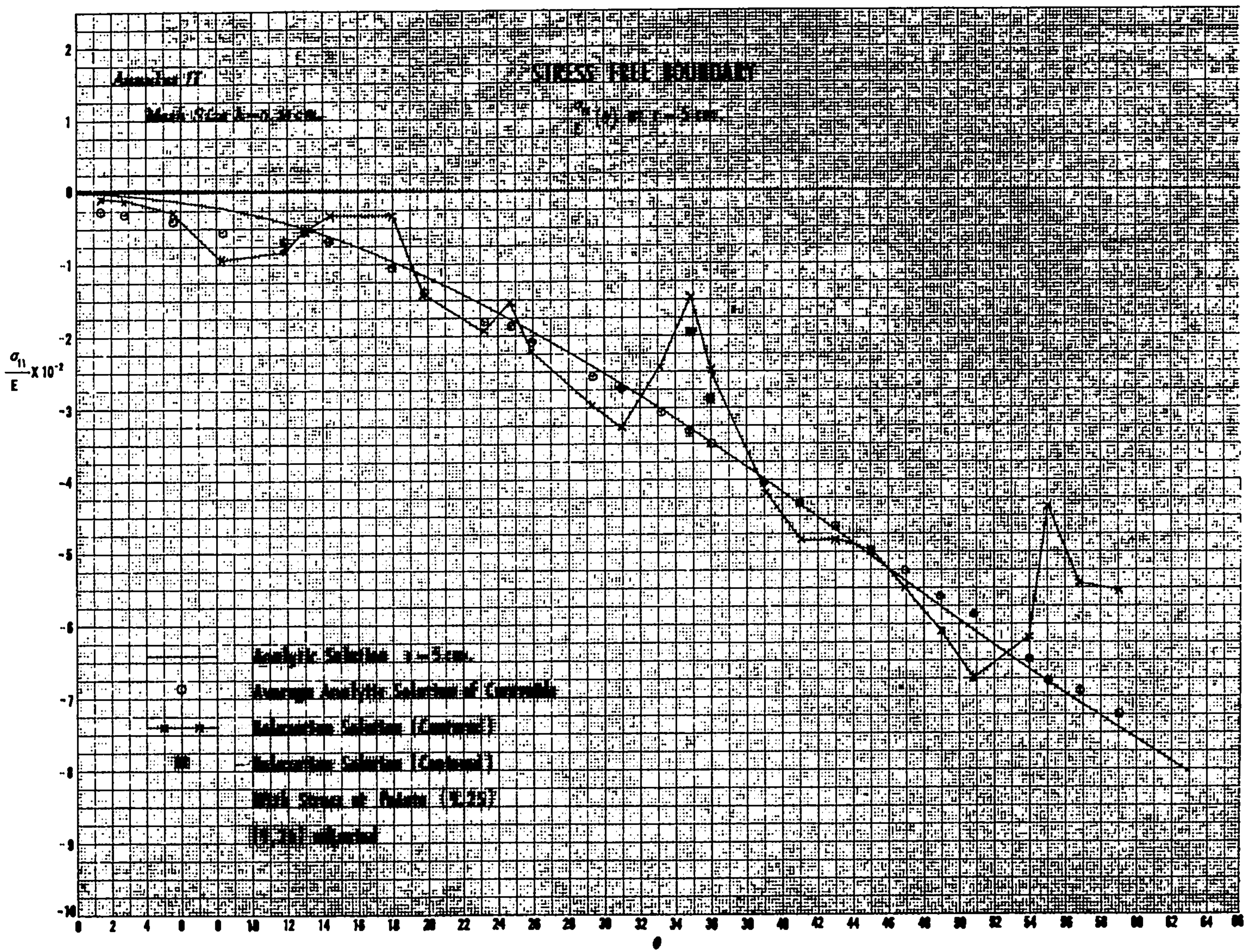

Figure 11. σ_{11} stress-free boundary

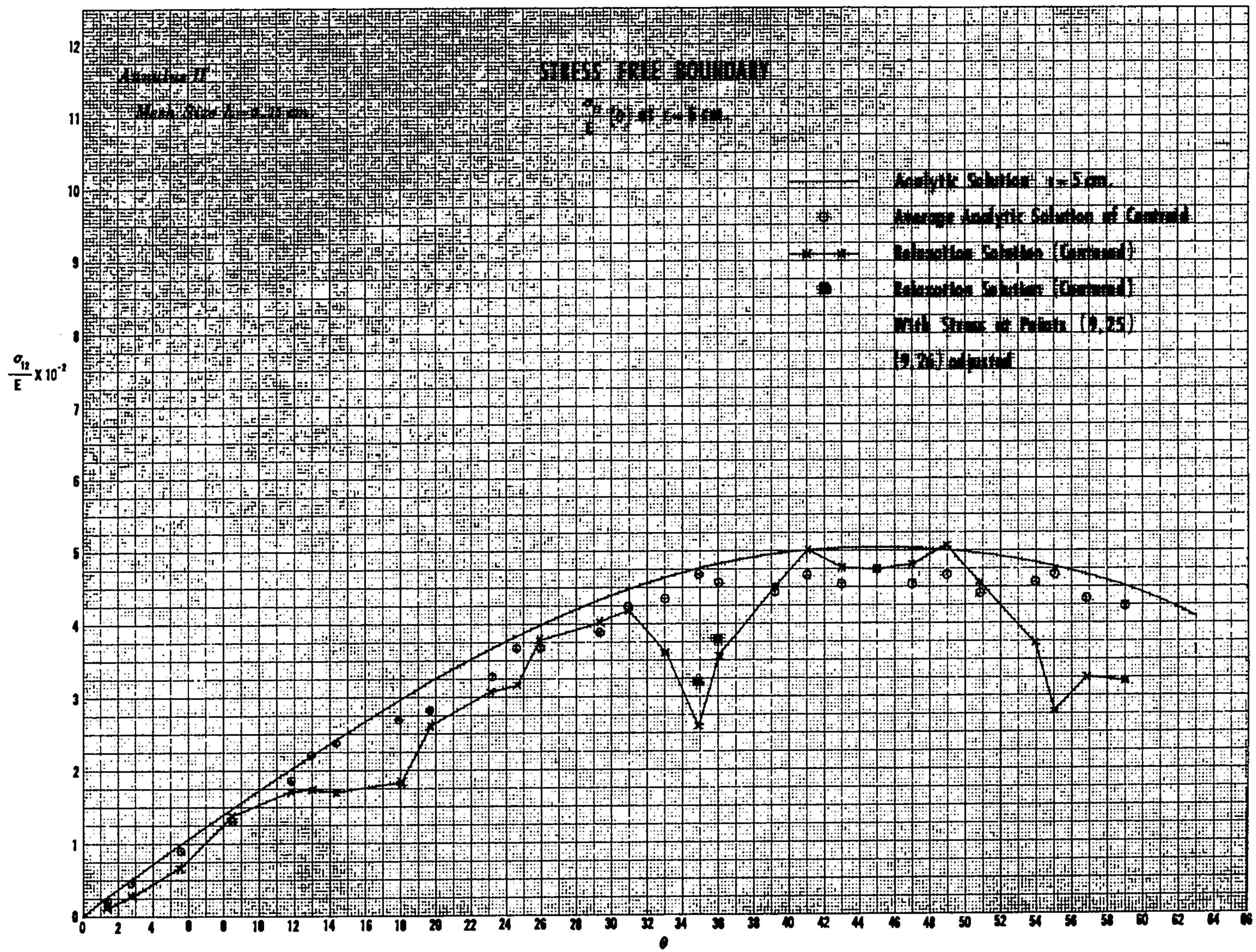

Figure 12. σ_{12} stress-free boundary

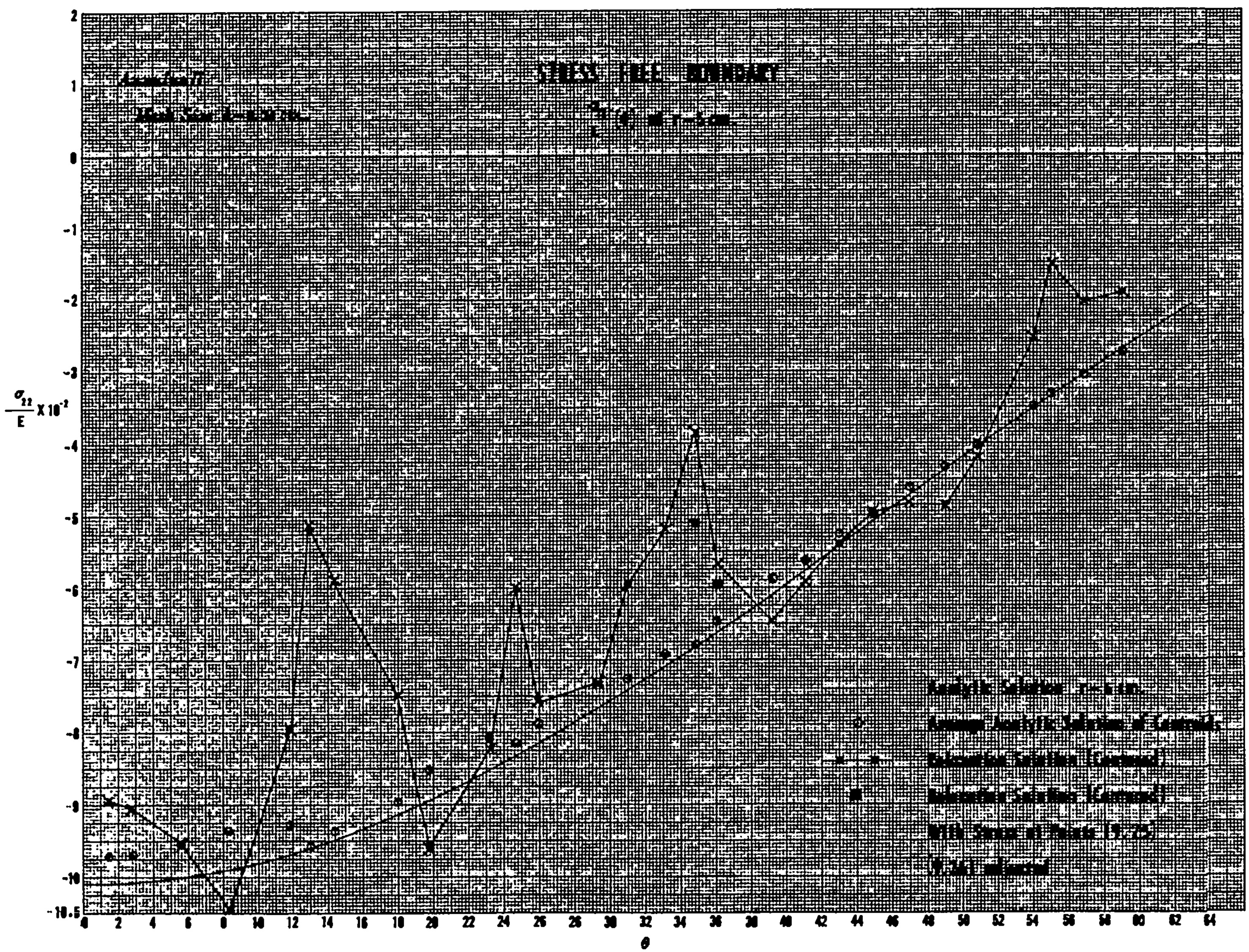

Figure 13. σ_{22} stress-free boundary

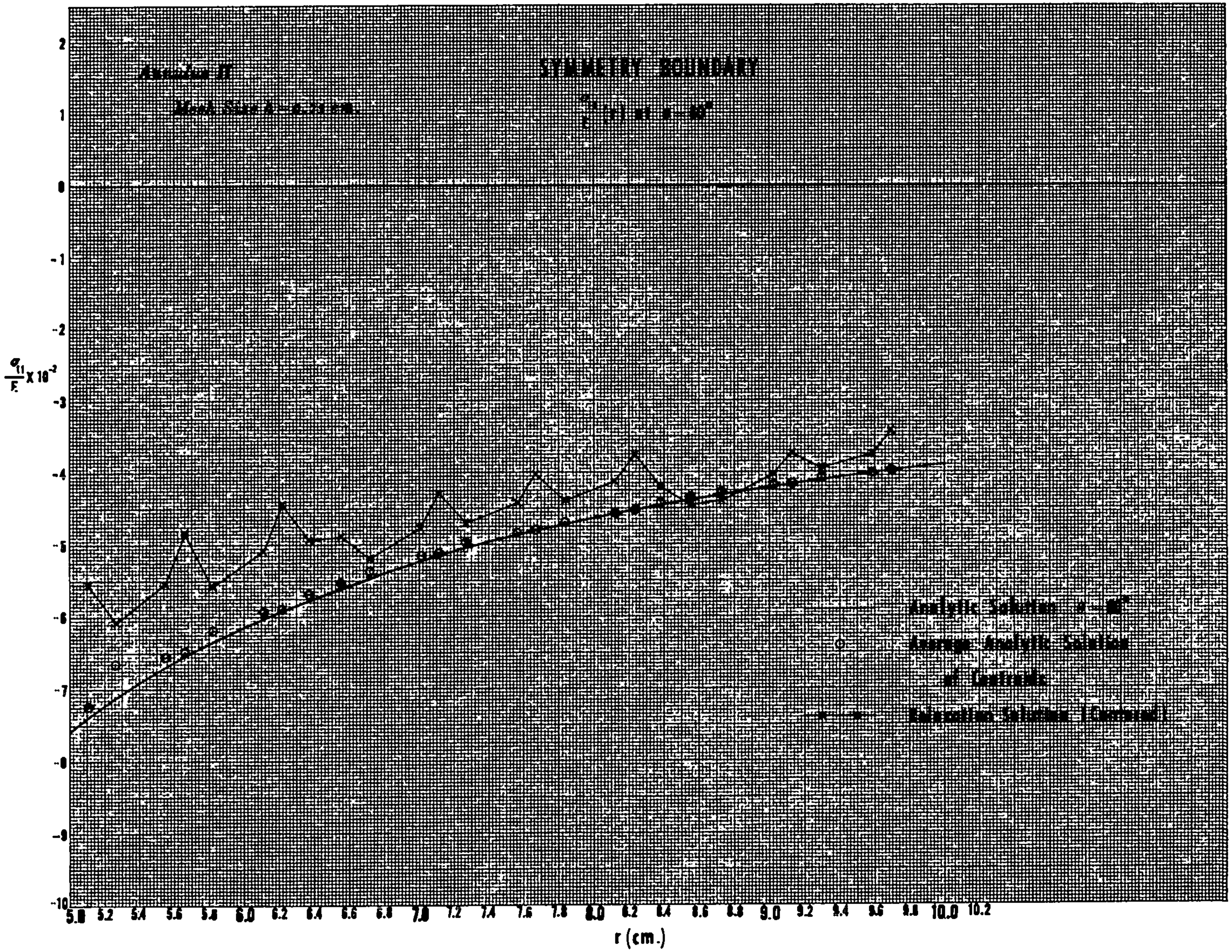

Figure 14. σ_{11} symmetry boundary, $\Theta = 60^{\circ}$

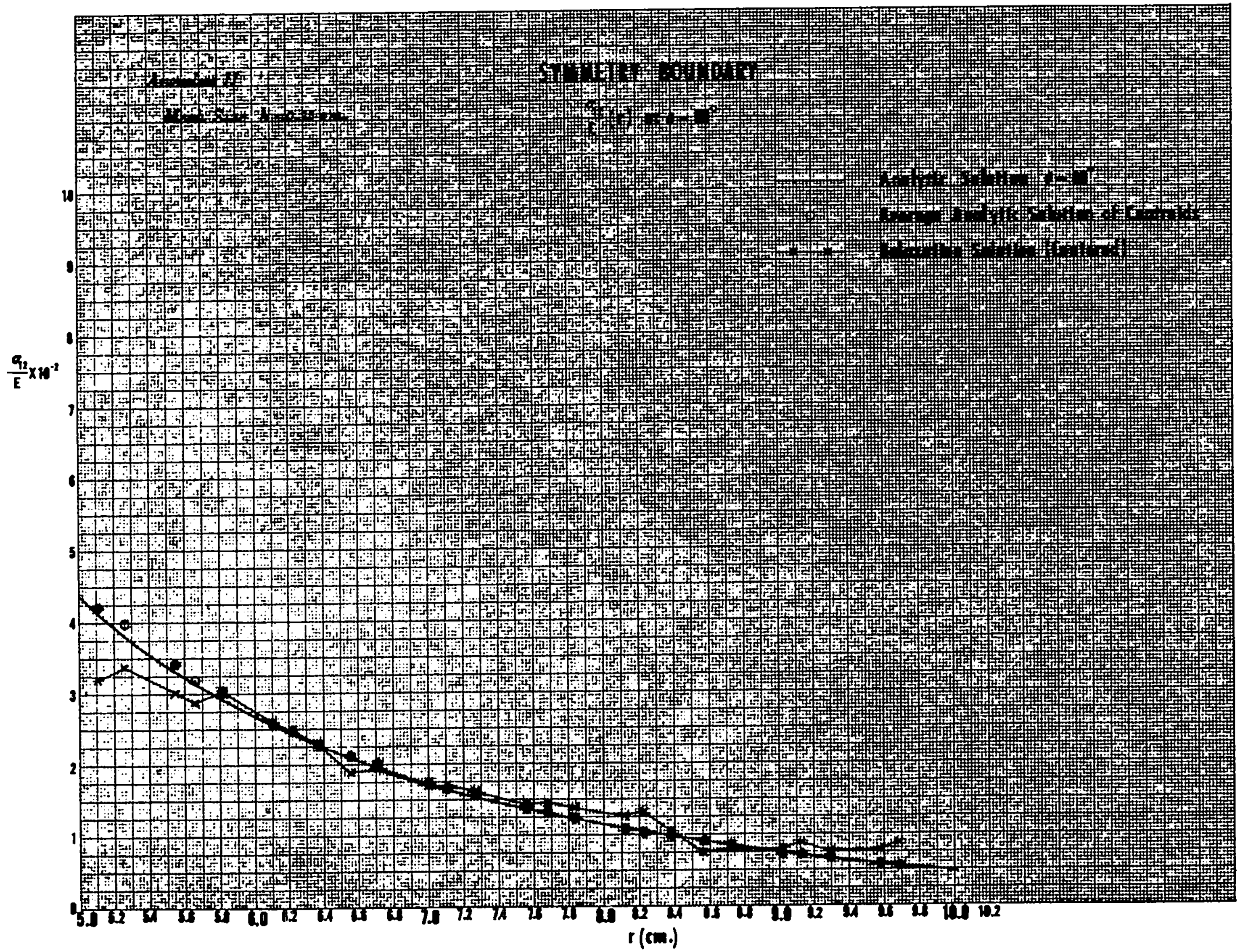

Figure 15. σ_{12} symmetry boundary, $\Theta = 60^{\circ}$

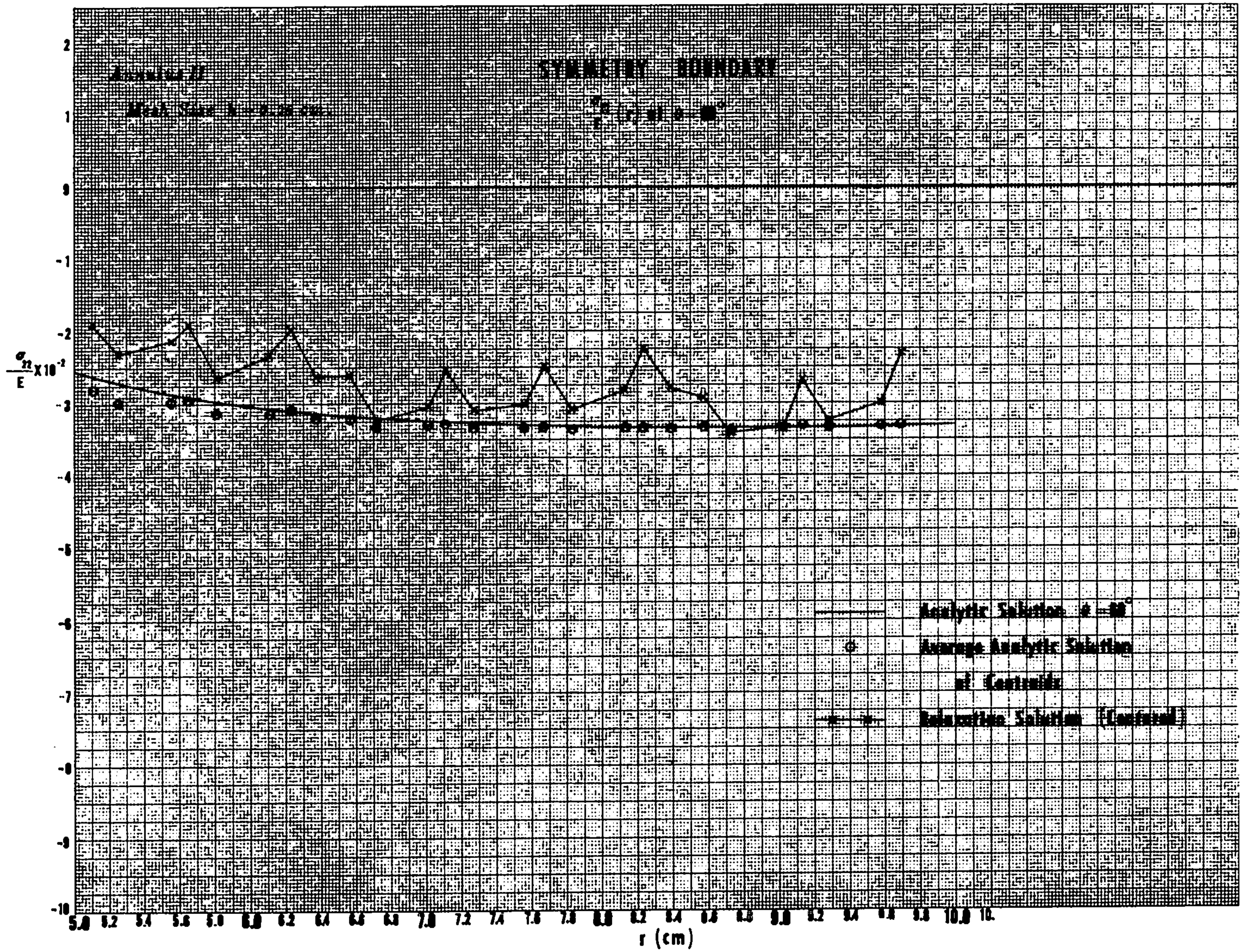

Figure 16. σ_{22} symmetry boundary, $\Theta = 60^{\circ}$

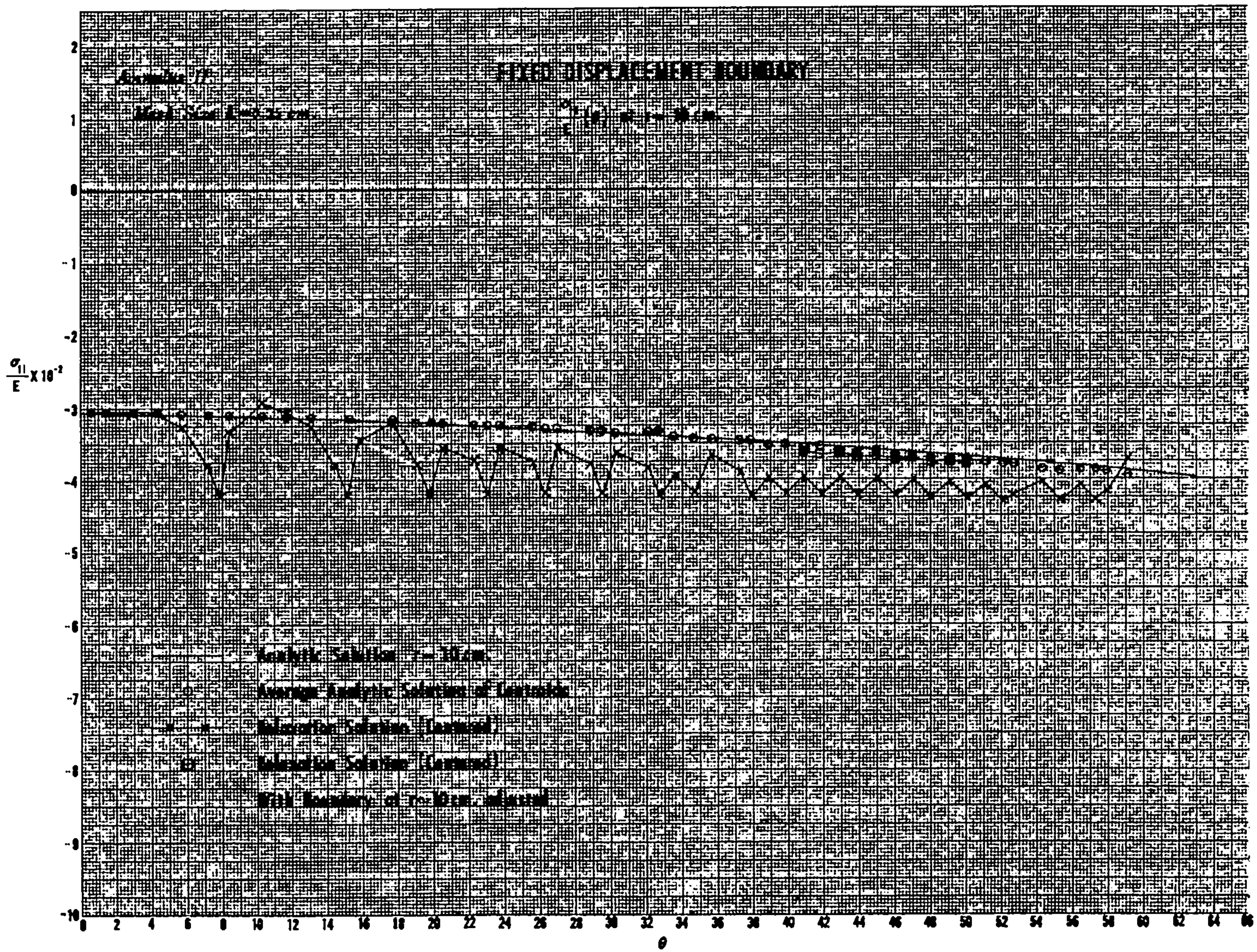

Figure 17. σ_{11} fixed displacement boundary

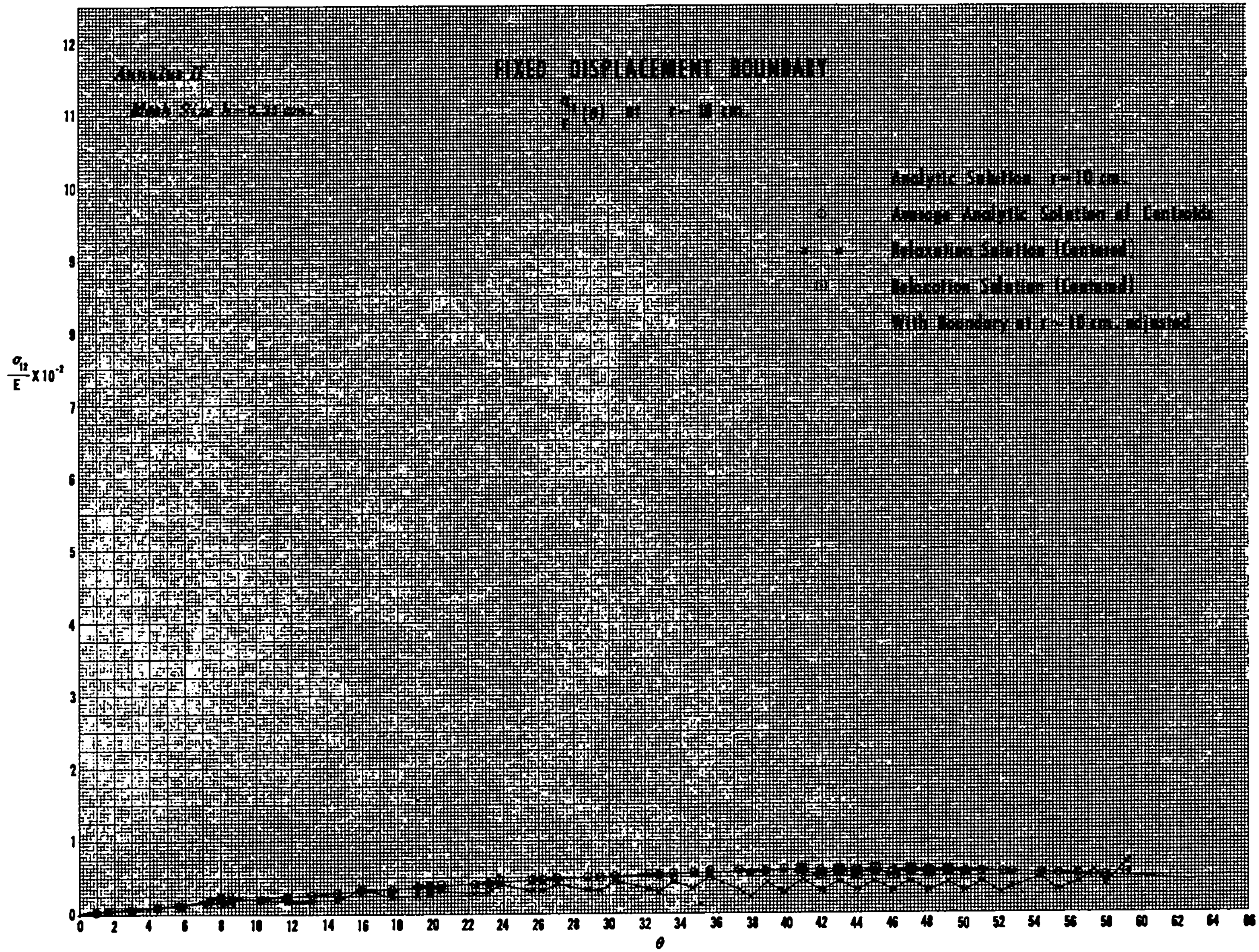

Figure 18. σ_{12} fixed displacement boundary

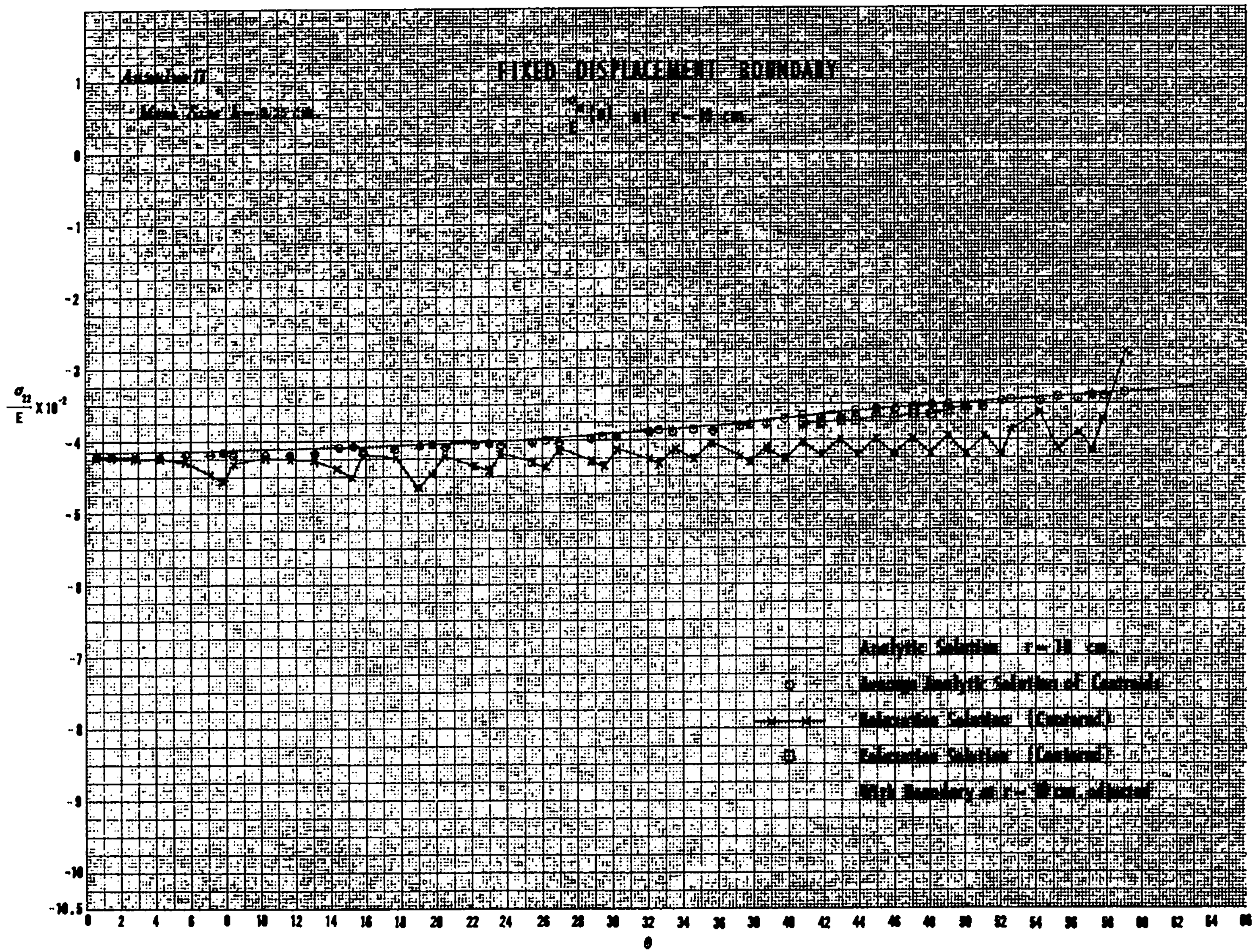

Figure 19. σ_{22} fixed displacement boundary

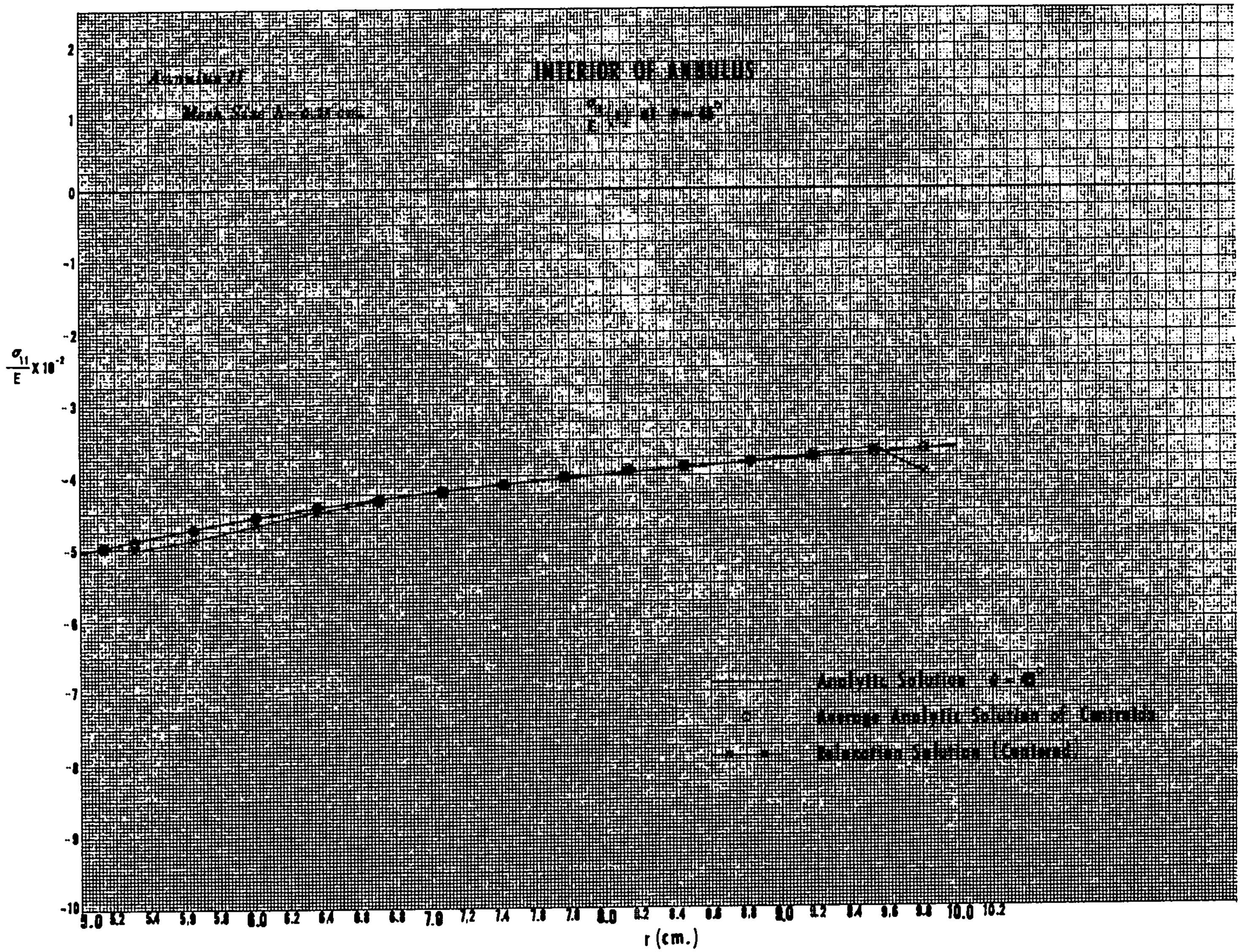

Figure 20. σ_{11} interior of annulus, $\theta = 45^\circ$

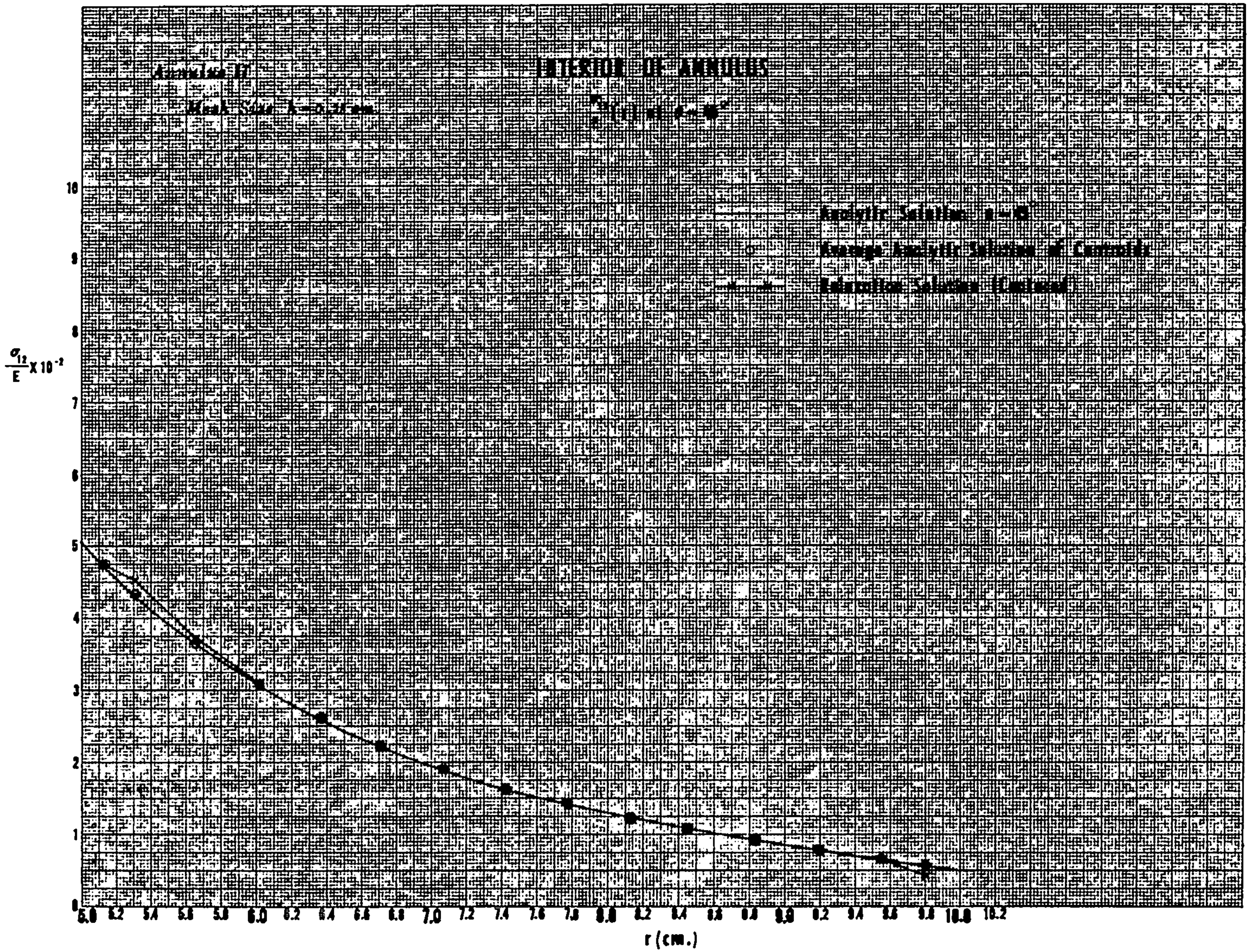

Figure 21. σ_{12} interior of annulus, $\Theta = 45^{\circ}$

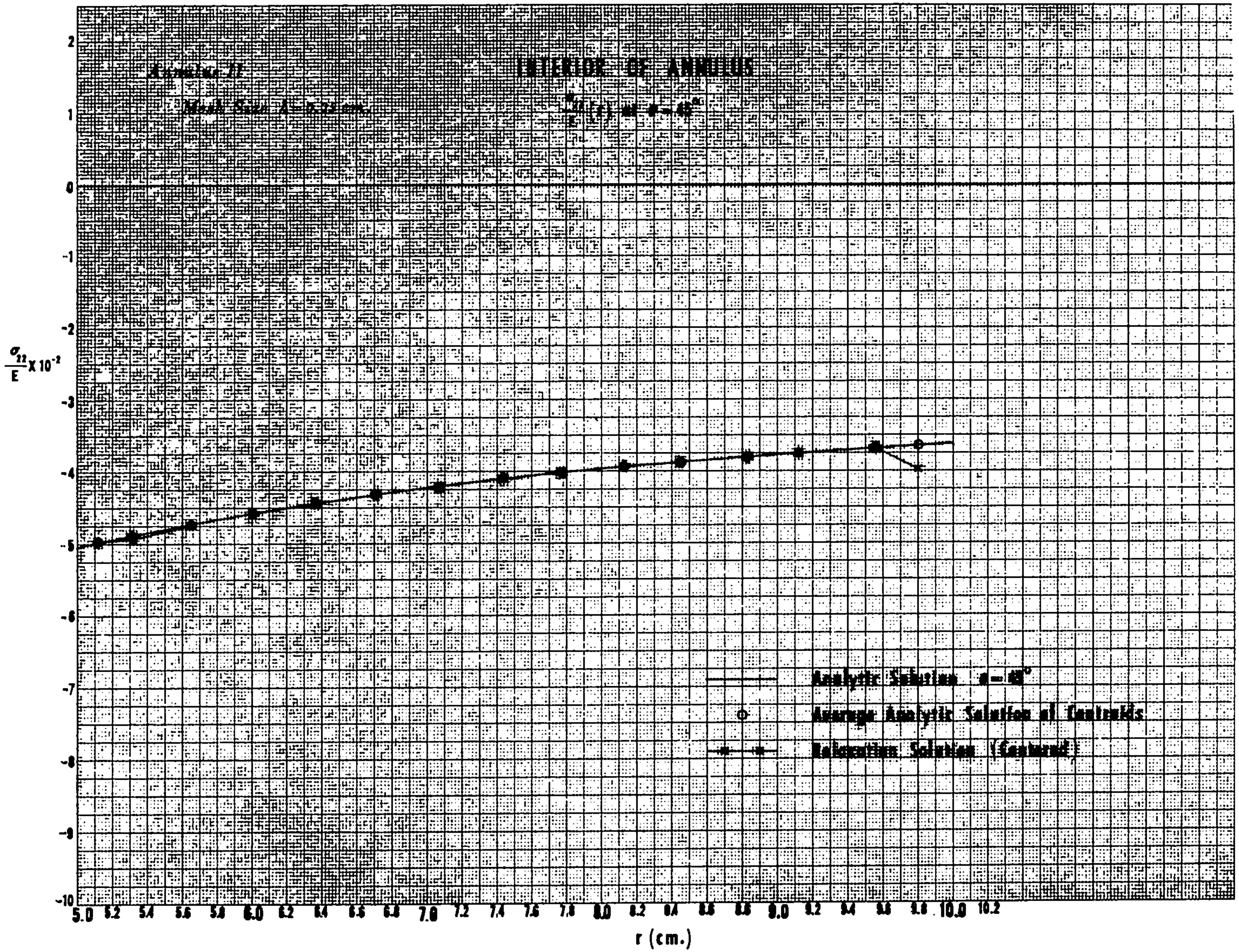

Figure 22. σ_{22} interior of annulus, $\theta = 45^{\circ}$