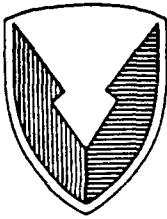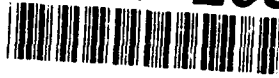AD-A255 203

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Numerical Analysis of Permittivity With Loss in Isotropic Binary Composites

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June 1992

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The use of composite materials and structures to provide characteristics unattainable directly from the constituent materials is well known. Work has been undertaken to apply this principle to the development of new dielectric materials for use in capacitors with greater energy density, lower loss, and higher breakdown resistance. This report describes the numerical analysis of permittivity in isotropic binary composite dielectrics through three-dimensional computer simulation.

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INTRODUCTION

The use of composite materials and structures to provide characteristics unattainable directly from the constituent materials is well known. Perhaps the most widespread example is steel-reinforced concrete wherein the high tensile strength of steel in conjunction with the high compressive strength of concrete yields a composite material with structural properties far superior to those of either constituent. More recently, work has been undertaken to apply this principle to the development of new dielectric materials for use in capacitors with greater energy density, lower loss, and higher breakdown resistance [1]. High permittivity dielectrics are necessary to achieve high energy densities, however high permittivity is usually associated with high loss. Low loss is similarly associated with low permittivity and low energy density dependent on loss tangent. Composite dielectrics of appropriate combinations of constituent materials may show high overall permittivity with small loss even though one or more of the constituents has large individual loss. This is known as the Maxwell-Wagner effect [2-4].

The net dielectric behavior of a randomly interspersed composite is dependent on the spatial dimensionality (1-D vs. 2-D vs. 3-D), domain geometries (domain size, domain shape, stratification, etc.), interconnection effects (percolation), and fractalization (interfaces or connectedness per unit volume). A self-similarity averaging law which is useful to the dielectric engineer is Lichtenecker's formula [5,6]

$$\epsilon^\alpha = \sum_k \epsilon_k^\alpha \ v_k \tag{1}$$

where ϵ is the resultant permittivity of the composite, α is an exponential averaging factor $(-1 < \alpha < +1)$, and the summation is over the constituent species with permittivity ϵ_k and volume fraction v_k respectively. This formula can be justified theoretically to apply to random (self-similar, scaleless) and history invariant composites. The permittivity ϵ is defined fully in terms of the electric and displacement fields and is frequency dependent. The factor α is referred to as the exponential averaging factor or self-similarity factor. The behavior of this factor has certain values in special limiting cases and was originally called a "formzahl" (form number) by Wiener [7]. In the case of isotropic flat layers with surface normals oriented parallel to the applied electric field, $\alpha = -1$, and for isotropic flat layers with surface normals perpendicular to the applied electric field direction, $\alpha = +1$. The mathematical interpretations of the exponential averaging factor for the following values are: $+1$ = 'arithmetic' averaging, 0 = 'geometric' (or logarithmic) averaging, and -1 = 'harmonic' averaging. In regard to the physical problem of randomly interspersed dielectric composites with a self-similarity, the values of the exponential averaging factor are only known to lie within these bounds [7-12]. The exponential averaging factor α however does offer a useful way of presenting results and general

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trends in a comparative sense to one another.

A second factor which is also bounded is the depolarization factor 'A'. The depolarization factor is a geometrical factor that arises from a self-consistent treatment of the dielectric problem where ellipsoidal domains are each surrounded by an effective medium host. This picture is usually the lowest order scattering approximation where the dielectric grains are much smaller than any associated electromagnetic wavelengths. The actual composite grains may be distant from the ellipsoidal shape, especially when dealing with mixtures not dominated strongly by any particular species. This approach is referred to as the effective-medium-theory coherent-potential-approximation (EMT-CPA) and has been derived in several manners [13-15]. It is most succinctly expressed as

$$\sum_k \frac{\epsilon_k - \epsilon}{A\epsilon_k - (1-A)\epsilon} v_k = 0 \ . \tag{2}$$

The depolarization factor 'A' can be determined by an integral which is taken over the shape of the ellipsoid and is discussed in Appendix A [11, 16-18]. In the case of a spheroid situated in N spatial dimensions the depolarization is simply $A = 1/N$.

Our analysis will be presented in both forms: the exponential averaging factor 'α' and the depolarization factor 'A'. The exponential averaging factor 'α' may be thought of as a measure of the degree between series and parallel-like extrema or Wiener bounds of the composite. The depolarization 'A' is a measure of geometric grain shape in terms of the effective-medium-theory coherent-potential-approximation (EMT-CPA). In the limit where the constituents of the composite are dielectrically infinitesimally close, the relation $\alpha \approx (1 - 2A)$ holds. It is interesting to note that equations (1) and (2) are first order approximations to each other in the close constituent permittivity limit even though the formulae appear quite different. However, when constituents having largely different permittivities are examined using our numerical program, the composite mixture formulae yield different predictions [1]. Both methods allow us to present our numerical simulation results in a comparative way which is useful for both theoretical and experimental analysis.

ELECTRIC DISPLACEMENT FIELD

The electric field $\mathbf{E}(\mathbf{r},t)$ is defined as the electric force per unit charge acting on a stationary test charge located at point $\mathbf{r}$ and at time t (Boldface notation will be employed throughout this report to represent vector and tensor quantities). The displacement field $\mathbf{D}(\mathbf{r},t)$ as used in this report is the universal displacement field which arises from the combination of Gauss's Law with charge continuity (conservation). The result is a continuous flux quantity. In the standard

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international (SI) MKSA unit format, these two relations are respectively

$$\nabla \cdot \mathbf{E}(\mathbf{r},t) = p_Q(\mathbf{r},t)/\epsilon_o \tag{3}$$

where $\nabla \cdot$ is the spatial divergence operator, $p_Q(\mathbf{r},t)$ is the volume charge density and ϵ_o is the permittivity of free space, and

$$\nabla \cdot \mathbf{J}_Q(\mathbf{r},t) = - dp_Q(\mathbf{r},t)/dt \tag{4}$$

where $\mathbf{J}_Q(\mathbf{r},t)$ is the charge current density (charge current per unit area). A generalized charge polarization field $\mathbf{P}_Q(\mathbf{r},t)$ is linked to the charge density by the following defining relation for $\mathbf{P}_Q(\mathbf{r},t)$

$$\nabla \cdot \mathbf{P}_Q(\mathbf{r},t) \equiv - p_Q(\mathbf{r},t) . \tag{5}$$

Upon partial time differentiation of equation (5) and comparing to the continuity equation (4) one finds the identity

$$\mathbf{P}_Q(\mathbf{r},t)/\ t = \mathbf{J}_Q(\mathbf{r},t) . \tag{6}$$

Segregation of charge types may be introduced when desired, but is not necessary for the derivation and application of a generalized permittivity [19] as in this report. A polarization field for discrete point charges in an inertial coordinate system from equation (5) could be

$$\mathbf{P}_Q(\mathbf{r},t) = \sum_i q_i \mathbf{r}_i . \tag{7}$$

In equation (7) the summation is over all charges q_i at locations $\mathbf{r}_i$ within the medium. Combining equation (3) and equation (5) yields

$$\{\epsilon_o \nabla \cdot \mathbf{E}(\mathbf{r},t) + \nabla \cdot \mathbf{P}_Q(\mathbf{r},t)\} = 0 . \tag{8}$$

Rearranging the brackets of equation (8) results in the divergence relation

$$\nabla \cdot \{\epsilon_o \mathbf{E}(\mathbf{r},t) + \mathbf{P}_Q(\mathbf{r},t)\} = 0 \tag{9}$$

or

$$\nabla \cdot \mathbf{D}(\mathbf{r},t) = 0 \tag{10}$$

where the quantity in the brackets becomes the definition of the generalized or universal electric displacement field [20]

$$\mathbf{D}(\mathbf{r},t) = \epsilon_o \mathbf{E}(\mathbf{r},t) + \mathbf{P}_Q(\mathbf{r},t) . \tag{11}$$

For brevity, this generalized field will be referred to as the 'D-field' elsewhere in this report. The time derivative of the D-field gives the generalized or universal displacement current density

$$\partial D(r,t)/\partial t = J_D(r,t) ,\tag{12}$$

referred to by Maxwell as the 'true current' and the D-field can be referred to as 'true' also [21]. From the combination of fundamental laws (3) and (4) with (11) and (12), it follows that the universal current density is always divergenceless and continuous with

$$\nabla \cdot J_D(r,t) = 0 .\tag{13}$$

Conversely, one might say that according to equation (12), the antiderivative (in time) of the universal current density is a vector field called the universal displacement field. The physical units of the displacement field are charge polarization per unit volume or that of surface charge density.

Dielectric measurements and analysis are often made in the frequency domain [22, 23]. In the case where the displacement field is periodic with time it can be Fourier decomposed as

$$D(r,t) = \int D(r,f) \ e^{+j2\pi ft} \ df\tag{14}$$

or conversely

$$D(r,f) = \int D(r,t) \ e^{-j2\pi ft} \ 2\pi \ dt\tag{15}$$

where $D(r,f)$ is the electric displacement field Fourier component at frequency f, $j \equiv \sqrt{-1}$, and integrations respectively are over all f and t. The frequency domain transformation of equation (10) gives

$$\nabla \cdot D(r,f) = 0 ,\tag{16}$$

or equivalently from combination of equations (12) and (13)

$$\nabla \cdot \{j \ 2\pi f \ D(r,f)\} = 0\tag{17}$$

for $f \neq 0$ (non-static fields). The relation expressed by equation (12) becomes in the frequency domain

$$j \ 2\pi f \ D(r,f) = J_D(r,f)\tag{18}$$

and so it is easy to transpose between equations (16) and (17).

In most natural media, the universal electric displacement field evolves by a collective decay from the past history of electric fields which are or have been impressed upon the medium. This is expressed by the convolution

$$D(r,t) = \int_{-\infty}^{t} f(r,t-t') \cdot E(r,t') \ dt'\tag{19}$$

or alternately upon change of integration variable to u defined as $u \equiv t-t'$,

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$$D(r,t) = \int_0^\infty \mathcal{F}(r,u) \cdot E(r,t-u) \, du \qquad (20)$$

where $D(r,t)$ is the displacement field at the present time, $E(r,t)$ is the electric field from the past to the present, the function $\mathcal{F}(r,u) = df(r,u)/du$ represents the history or decay correlation between the fields and $u \equiv t-t'$ is the present to past time connection variable. The function $\mathcal{F}(r,u)$ is referred to as the normalized displacement decay current or, in short, decay current. The accumulation of normalized displacement decay current is called the normalized displacement decay function $f(r,u)$ or, in short, decay function. The dimensions of the decay function $f(r,u)$ are displacement field per electric field. Causality requires that the decay current $\mathcal{F}(r,t-t')$ be zero when $t' > t$ or $u < 0$ (i.e., no correlation with the future). In the time domain both the displacement and electric fields must be real valued and hence the normalized displacement decay current $\mathcal{F}(r,u)$ must also be real valued. If the medium is linear then the decay current $\mathcal{F}(r,u)$ is independent of the electric field in the medium. For example if the decay function $f(r,u)$ is just a step function (from zero) at $u = t-t' = 0$ then equations (19) and (20) reproduce an instantaneous correlation between the electric and displacement fields. In the next section we will discuss the implications of these physical constraints upon dielectric permittivity behavior.

In summary, a universal electric displacement field or 'D-field' can be defined which is inclusive of all charges. This generalized D-field is necessary for use in dielectric composites. Provided there are no unaccounted for sources, sinks, or charge accumulations, then this field is divergenceless and continuous. A normalized displacement decay current/function can be introduced to statistically relate the present observed displacement field to the past electric field history.

DIELECTRIC PERMITTIVITY

Dielectric permittivity is defined by a tensor relationship between the electric and displacement field vectors in the frequency domain which may be expressed as

$$D(r,f) = \epsilon(r,f) \cdot E(r,f) \qquad (21)$$

where $E(r,f)$ and $D(r,f)$ are respectively the electric and universal displacement fields at a location r and frequency f. Alternately this relationship can be expressed using spatial index notation

$$D_i(r,f) = \epsilon_{ij}(r,f) \, E_j(r,f) \; . \qquad (22)$$

The dielectric permittivity $\epsilon_{ij}(r,f)$ is a tensor of rank two.

The dielectric permittivity is defined in the frequency regime because, strictly speaking, there are no known substances

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(except vacuum) which exhibit complete instantaneous displacement response to the application of an electric field. The implication of this fact is that there are no completely static time domain constants between electric and displacement fields. Rather there exists a time correlation behavior between the present displacement field and the past applied electric fields. This is expressed by equations (19) and (20) and the normalized displacement decay current $\dot{f}(r,t-t')$ or through its accumulation as the normalized displacement decay function $f(r,t-t')$. The frequency domain transformation of the convolution relation expressed by equations (19) and (20) produces the needed relation connecting the frequency domain permittivity $\epsilon(r,f)$ with the normalized displacement decay current $\dot{f}(r,t-t')$ of the time domain as

$$\epsilon(r,f) = \int_0^\infty \dot{f}(r,u) \, e^{+j2\pi fu} \, du \qquad (23)$$

where the time variable is $u = t-t'$. Because the decay current and decay function are real valued, the frequency domain permittivity $\epsilon(r,f)$ is necessarily complex valued unless the decay function is instantaneous. Traditionally, in the field of dielectrics, this is expressed as

$$\epsilon(r,f) = \epsilon'(r,f) + j \, \epsilon''(r,f) \qquad (24)$$

where $\epsilon'(r,f)$ and $\epsilon''(r,f)$ are respectively the real and imaginary parts of the dielectric permittivity. The imaginary part of permittivity is known as the "lossy" part as it is proportional to the energy lost during a cycle of a time harmonic field.

When a medium is isotropic, both the displacement and electric field vectors are colinear and the permittivity can be regarded as the scalar ratio $\epsilon(r,f)$ of the fields $D(r,f)/E(r,f)$. In situations where the medium is anisotropic or birefringent, then the fields are reoriented locally until they lie along the direction of a principal axis of the local permittivity tensor. In this alignment the fields are colinear and their ratio can be measured as before as the corresponding element in the diagonalized permittivity tensor. In the general anisotropic situation where the principal directions may not experimentally be possible to determine, measurements have to be made of all spatial aspects pertaining to both field vectors. For isotropic dielectrics where the permittivities are scalar and spatially uniform, the ratio of the imaginary to real part of the permittivity is called the loss tangent or dissipation factor [24, 25]. This is conventionally written as

$$\epsilon''(r,f)/\epsilon'(r,f) \equiv \tan \delta(r,f) . \qquad (25)$$

In this report we will examine the case of random (Monte Carlo) composite media simulations with a high degree of macroscopic isotropy. Expansion to anisotropic cases is anticipated in future work.

As an illustrative case, when the decay function is isotropic and spatially uniform with an exponential decay $f(t) = \epsilon_A (1 - e^{-t/T})$ (reflecting a viscous type relaxation), it transforms into the familiar simple form of Debye relaxation

$$\epsilon(f) = \int_0^\infty (\epsilon_A/T)(e^{-t/T})(e^{+j2\pi fu}) \, du \tag{26}$$

$$\epsilon(f) = \epsilon_A/(1 - j2\pi fT) \tag{27}$$

where ϵ_A is the transition permittivity (a constant), and T is the viscous relaxation time. Note that $\epsilon(f)$ here is a complex numbered quantity expressible as the real and imaginary pair

$$\epsilon'(f) = \epsilon_A/[1 + (2\pi fT)^2] \tag{28}$$

and

$$\epsilon''(f) = \epsilon_A \, 2\pi fT/[1 + (2\pi fT)^2] \, . \tag{29}$$

An interesting feature of the Debye relaxation permittivity is that the complex plane plot of $\epsilon'(f)$ and $\epsilon''(f)$ reveals a semicircle as frequency is varied. This type of plot is often referred to as the Cole-Cole plot and is useful as a way of identifying the relaxation as well as fingerprinting permittivity characteristics. Elimination of the explicit frequency variable on the right hand sides of the above equation pair does indeed verify a semicircle of radius $\epsilon_A/2$ whose imaginary part reaches its maximum value when the frequency is at $1/2\pi T$.

CONDUCTIVITY

A universal displacement conductivity $\sigma(r,f)$ is defined by a tensor relationship between the electric field and universal displacement current density vectors in the frequency domain as

$$J_D(r,f) = \sigma(r,f) \cdot E(r,f) \, . \tag{30}$$

Combining equations (18), (21), and (30) yields

$$\sigma(r,f)/j2\pi f = \epsilon(r,f) \tag{31}$$

as the connection of the universal displacement conductivity and the universal permittivity subject to the constraint that $f \neq 0$. The convolution for universal displacement conductivity becomes

$$\sigma(r,f) = j2\pi f \int_0^\infty f(r,u) \, e^{+j2\pi fu} \, du \, . \tag{32}$$

The universal displacement conductivity as a complex number can be expressed in terms of its real and imaginary parts as

$$\sigma(r,f) = \sigma'(r,f) - j \, \sigma''(r,f) \tag{33}$$

where $\sigma'(r,f)$ and $\sigma''(r,f)$ are respectively the real and imaginary parts. The direct current (DC) conductivity is the limiting case

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of the real part of the conductivity when the frequency tends toward zero. However the projected value of DC conductivity becomes less distinct when nonstatic measurements are made at higher and higher frequencies especially over a limited bandwidth.

Exploiting the identity posed by equation (31) yields

$$\sigma'(r,f) = 2\pi f\ \epsilon''(r,f) \tag{34}$$

and

$$\sigma''(r,f) = 2\pi f\ \epsilon'(r,f)\ . \tag{35}$$

When a medium is isotropic, the displacement current density $J_D(r,f)$ and electric field $E(r,f)$ vectors are colinear. In this instance, the universal displacement conductivity can be regarded as the scalar ratio $\sigma(r,f)$ of vectors given by $J_D(r,f)/E(r,f)$. If the medium is anisotropic or birefringent, then one may reorient alongside a principal axis of the local conductivity tensor to determine the tensor components. The loss tangent defined in equation (25) becomes

$$\tan \delta(r,f) = \sigma'(r,f)/\sigma''(r,f)\ . \tag{36}$$

in terms of the real and complex conductivity parts.

CAUSALITY

A physical response is said to be causal if it occurs at or following an excitation. In classical systems most responses cannot anticipate future excitations and hence their connecting functions are null. A partial relaxation of this behavior may occur in quantum mechanical systems wherein the connecting function becomes a probability. Quantum mechanical causality or other non-local overlapping shall not be dealt with in this report. Both frequency domain universal dielectric permittivity $\epsilon(r,f)$ and conductivity $\sigma(r,f)$ arise from a causal function. This function is the time domain normalized displacement decay current $\dot{f}(r,u)$ or alternately, its accumulation, the normalized displacement decay function $f(r,u)$. The time variable u is the difference between present and past times u = t-t'. The decay function is a time domain function and it must be zero when u is negative (a non-zero value would indicate future excitations that cannot have happened yet). The decay function relates real-valued physical vector quantities over past history as specified in the convolution equations (19) and (20). The consequence is that the decay function and permittivity are related by transformation equation (23). The inverse relation that obtains the decay function from the permittivity spectrum exists and is required to possess the aforementioned physical constraints. The inversion procedure is accomplished by means of complex Laplace transforms or equivalently unilateral/one-sided Fourier transforms. This procedure requires that the frequency be

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treated as a complex number which can be viewed as lying in the complex frequency ('s') plane. The complex frequency is defined as

$$s \equiv -j2\pi f \; . \tag{37}$$

The substitution of the variable s into equation (23) leads to the alternate expression for the permittivity

$$\epsilon(r,s) = \int_0^\infty \mathcal{F}(r,u) \; e^{-su} \; du \tag{38}$$

where the other variables are the same as before. In Laplace transform operator notation equation (38) can be succinctly written as

$$\epsilon(r,s) = \mathcal{L}(\mathcal{F}(r,u)) \tag{39}$$

where $\mathcal{L}$ denotes the Laplace integral transform operation $\int_0^\infty [...] \; e^{-su} \; du$ acting upon $\mathcal{F}(r,u)$. The inverse operation can be obtained through residue theory and is

$$\mathcal{F}(r,u) = \frac{1}{2\pi j} \int_{+c-j\infty}^{+c+j\infty} e^{+su} \; \epsilon(r,s) \; du \tag{40}$$

where the contour c is chosen such that all the singular points of $\epsilon(r,s)$ lie to the left of the contour on the s-plane. In Laplace operator notation one can simply write equation (40) as

$$\mathcal{F}(r,u) = \mathcal{L}^{-1}(\epsilon(r,s)) \tag{41}$$

where $\mathcal{L}^{-1}$ denotes the inverse Laplace transform as given in the expression (39).

The significance of these transformation expressions between the permittivity and decay function is that of two important properties: 1) complex conjugation, and 2) analyticity and interdependence between real and imaginary parts. These two properties are of consequence to dielectric observation.

1) The property of complex conjugation requires that the permittivity (as well as conductivity) become complex conjugate whenever the s-frequency becomes conjugate, i.e.

$$\epsilon^*(r,s) = \epsilon(r,s^*) \; , \tag{42}$$

where the asterisk superscript denotes conjugation of the preceding variable. The relationship expressed by equation (42) can be inferred by complex conjugation of the s-frequency in the transformation relations, (38) through (41). Graphically, on the s-plane the real parts of the permittivity and conductivity functions are mirror symmetric about the real s-axis, while the imaginary parts are antisymmetric about the real s-axis. This property not only allows complex conjugation to occur between

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physicists and electrical engineers, i.e., $j = -i$, but also applies whenever a dielectric permittivity may be made up of functions which are functions of complex frequency. This occurs, for example, in the case of composite mixtures. Therefore the action of applying composite mixture relations to well-behaved constituents cannot introduce any violations of the conjugation property in the resultant dielectric response.

2)   The second property of analyticity and real/imaginary parts interdependence is commonly referred to as the Kramers-Kronig relationship [23, 26-28]. This relationship can be stated in different forms such as a pair of complementary Hilbert transforms or as a pair of one-sided integrals between the real and imaginary parts of permittivity or conductivity. The Kramers-Kronig relationship is manifested in the analyticity (i.e., Cauchy-Riemann conditions) and lack of singularities of the permittivity function on the right side (positive s-values, real part) of the s-plane. If a singularity occurs on this portion of the s-plane, then an unstable or undefined dielectric system response would occur at some range of physically realizable excitation frequencies. In order that the decay function $f(\mathbf{r},u)$ consistently remains causal and real valued, then the singularities can only exist on the left side of the s-plane either on the negative real s-axis or as complex conjugate pairs on the left side (negative s-values, real part) of the s-plane. The Kramers-Kronig relation for permittivity may be written

$$\epsilon(\mathbf{r},s) = \frac{-j}{\pi} \oint_c \frac{\epsilon(\mathbf{r},z)}{z-s} \, dz \qquad (43)$$

where the integral is principal valued with the contour c running first along the imaginary s-axis from negative to positive then clockwise in a large semicircle about the right half s-plane. The variable z is a variable of integration. Using the complex conjugation property of equation (42) and reverting back to the ordinary frequency notation f, the Kramers-Kronig relation can be written as the integral pair

$$\epsilon'(\mathbf{r},f) = \frac{2}{\pi} \int_0^\infty \frac{f' \, \epsilon''(\mathbf{r},f')}{(f'^2-f^2)} \, df' \qquad (44)$$

and

$$\epsilon''(\mathbf{r},f) = \frac{2f}{\pi} \int_0^\infty \frac{\epsilon'(\mathbf{r},f')}{(f'^2-f^2)} \, df' \, . \qquad (45)$$

Kramers-Kronig requirements also apply to composite mixture permittivities in that the mixing relations cannot introduce contradictions to well-behaved constituents.

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MACROSCOPIC DIELECTRIC QUANTITIES

Both composite dielectric analysis and dielectric data acquisition are carried out over regions of finite spatial extent. Dielectric data acquisition can be a formidable task because of a limited ability to resolve the electric and displacement field vector components, as well as other considerations such as extraneous polarizations and stray fields.

Macroscopic quantities must be introduced such that the overall displacement flux remains continuous. The conversion can be accomplished in going from the differential form equation (10) (Gauss' law) into an integral form via the divergence theorem of mathematics as

$$\int_v \mathbf{\nabla} \cdot \mathbf{D}(\mathbf{r},t) \ dr^3 = \int_v 0 \ dr^3 \qquad (46)$$

and

$$\oint_a \mathbf{D}(\mathbf{r},t) \cdot \hat{n} \ dr^2 = 0 \ . \qquad (47)$$

In equation (46), the integration is performed over the volume v enclosed by a closed surface. In equation (47), the integration is taken over the surface enclosing volume v, and $\hat{n}$ is the outward drawn surface normal unit vector. We can conveniently restate equation (47) in terms of a universal displacement flux Φ corresponding to the integrated displacement field passing through a given surface. This may be written in the time domain as

$$\Phi_n(t) \equiv \int \mathbf{D}(\mathbf{r},t) \cdot \hat{n} \ dr^2 \qquad (48)$$

or in the frequency domain as

$$\Phi_n(f) \equiv \int \mathbf{D}(\mathbf{r},f) \cdot \hat{n} \ dr^2 \qquad (49)$$

with the integral taken over the area of the surface in question. In terms of displacement flux Φ, the integral form of equation (47) becomes

$$\oint_a d\Phi(\mathbf{r},t) = 0 \qquad (50)$$

in the time domain or

$$\oint_a d\Phi(\mathbf{r},f) = 0 \qquad (51)$$

in the frequency domain. In equations (50) and (51), $d\Phi(\mathbf{r},t)$ and $d\Phi(\mathbf{r},f)$ denote the incremental displacement flux as the integration proceeds around the closed surface. The right hand sides of equations (50) and (51) are zero for this universal form of electric displacement because we have chosen the displacement to be inclusive of all charges and an overall charge neutrality exists within the enclosure. The units of displacement flux Φ are that of charge. The time derivative of displacement flux

possesses units of charge current. Equations (50) and (51) are
thus simply a statement of charge/displacement field continuity
and conservation. The interpretation of an electric displacement
field flux is that a flux originates or terminates on a charge of
that value.

The conversion of equations (10) and (16) into the integral
equations (50) and (51) requires the choice of some enclosing
'Gaussian' surface. Generally this choice is that of convenience
over which the macroscopic permittivity ϵ(f) is defined. The
macroscopic permittivity is defined in the same sense as the
microscopic permittivity of equations (21) and (22) with the
distinction that the field quantities are mean valued over the
volume of the enclosure. The defining relation for the
macroscopic permittivity tensor ϵ(f) becomes

$$D(f) = \epsilon(f) \cdot E(f) \tag{52}$$

where $D(f)$ and $E(f)$ are respectively the mean valued displacement
and electric fields over the selected 'Gaussian' enclosure.
Since the permittivity or conductivity is always defined in the
context of the frequency domain, for the remainder of this report
we will drop the explicit frequency dependence notation with the
understanding that the frequency dependence does remain. Thus in
this reduced shorthand notation the permittivity ϵ is

$$D = \epsilon \cdot E \tag{53}$$

where again D and E are respectively the displacement and
electric fields understood to be macroscopic and of the frequency
domain. The macroscopic versions of other relevant dielectric
relations are as follows:

i)   The evolution from a decay function corresponding to
equation (23) is

$$\epsilon = \int_0^\infty f(u) \, e^{+j2\pi fu} \, du \tag{54}$$

where ϵ is the macroscopic permittivity (frequency dependent) and
$f(u)$ is the normalized macroscopic displacement decay current.
The integration is performed over all past times u at fixed
frequency f.

ii)   The macroscopic permittivity is expressible in terms of its
real and imaginary parts as in equation (24) as

$$\epsilon = \epsilon' + j \, \epsilon'' \, . \tag{55}$$

iii) The loss tangent for the macroscopic and isotropic
dielectric specimen is the ratio of the imaginary to real
permittivity portions

$$\tan \delta \equiv \epsilon''/\epsilon' \, . \tag{56}$$

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iv)   The displacement current conductivity in the macroscopic case is found from equation (30) to be

$$\mathbf{J}_D = \boldsymbol{\sigma} \cdot \mathbf{E} \qquad (57)$$

where $\mathbf{E}$ is the electric field and $\mathbf{J}_D = \partial \mathbf{D}/\partial t$ is the universal displacement current density at a given frequency.

v)   The relation between the macroscopic permittivity and conductivity is found from equation (31) to be

$$\sigma/j2\pi f = \epsilon . \qquad (58)$$

vi)   The macroscopic conductivity can be separated into its real and imaginary parts as

$$\sigma = \sigma' - j\,\sigma'' . \qquad (59)$$

vii) When the medium is isotropic with respect to the macroscopic permittivity, it also must be isotropic in the displacement conductivity and thus the loss tangent given by

$$\tan \delta = \sigma'/\sigma'' \qquad (60)$$

can be found in similar fashion to that of equation (36).

viii) A macroscopic medium obeys causality and its behavior is derivable as an analytic function through the use of Laplace transform techniques upon the normalized displacement decay current. In Laplace operator notation we can write

$$\epsilon(s) = \pounds(\mathfrak{f}(u)) \qquad (61)$$

where $\pounds$ denotes the Laplace integral transform operation $\int_0^\infty [\dots] e^{-su} du$ acting upon $\mathfrak{f}(u)$.

ix)   The complex conjugation property demands that a causal analytic function which stems from a real valued time function obey

$$\epsilon^*(s) = \epsilon(s^*) . \qquad (62)$$

The complex conjugation property imposes a restriction on the choice of composite mixture formulae. Application of this property to the kth constituent species and considering that the composite response also must be causal results in

$$\epsilon^* = f\{\epsilon_1^*, \epsilon_2^*, \epsilon_3^*, \dots \epsilon_k^*, \dots\} \qquad (63)$$

where ϵ^* is the conjugate permittivity of the composite, ϵ_k^* is the conjugate permittivity of the kth constituent species, and f denotes some functional.

x)   The Kramers-Kronig relation expresses the interdependence

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between the real and imaginary parts as

$$\epsilon(s) = \frac{-j}{\pi} \int_C \frac{\epsilon(z)}{z-s} \, dz \qquad (64)$$

where the integral is principal valued with the contour c running first along the imaginary s-axis from negative to positive then clockwise in a large semicircle about the right half s-plane. The variable z is a variable of integration. Such a relationship is of use in determining valid composite mixture formulae and for checking authenticity or filling in data gaps.

The interrelations expressed or implied in i) through x) for a macroscopic dielectric specimen are valid providing the macroscopic 'Gaussian' enclosure boundaries do not change.

DIELECTRIC COMPOSITE MIXTURE FORMULAE

Knowledge of the dielectric characteristics such as permittivity for a particular macroscopic configuration does not imply full knowledge of the subassembly of possible microscopic configurations. This degeneracy exists whenever a dielectric medium is nonuniform such as in the case of composites. This degeneracy even already exists for a simple composite constructed of stratified flat layers with fixed constituent volume fractions. In this special case, the solution can be worked out with treatment as a collection of capacitors aligned either in series or parallel [4, 29].

As a consequence, there can exist a set of composite mixture formulae which will satisfy or nearly satisfy a given particular macroscopic dielectric observation. Evidence of such degeneracy of formulae can be found in some of reviews on composite mixtures [25, 30-34]. Moreover, the wavelengths of the probing fields typically applied in dielectric measurements generally are not capable of resolving microscopic features and therefore the measured macroscopic response can only reflect collective behaviors.

One criterion for the applicability of a particular composite mixture formula is that the dielectric response predicted for a composite cannot introduce any new information, particularly in regard to microscopic configurations. In the case of random composites there is by definition a lack of specific knowledge of microscopic configurations and in order for a mixture formula to be of relevance it must contain a minimum of parameters pertaining to the microscopic configuration. The composite dielectric response predicted by a mixture formula must also reflect the same symmetry properties that are posed by the physical input situation.

Two mixture formulae can be shown to be particularly applicable to the case of random dielectric composites, namely

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Lichtenecker's formula as given in equation (1) and the EMT-CPA formula as given in equation (2). Each of these two composite mixture formulae can be explained with reference to their constraints and applicability, as follows:

I)   The Lichtenecker's dielectric mixture formula of equation (1) is a self-similarity formula derivable by a process of constraint elimination starting with a generalized expression [5, 6]. The several constraining arguments are:

1)   Proportionality and role symmetry must be maintained between the resultant outcome and that obtained when all the constituents are changed by the same common factor. Mathematically this may be stated as

$$m\epsilon = g[m\epsilon_1, m\epsilon_2, m\epsilon_3, \ldots] \tag{65}$$

where m is a real multiplicative factor, g means a generalized functional, ϵ is the composite permittivity, ϵ_1 is the permittivity of constituent species 1, etc.. The role symmetry argument implies that no one constituent be different than any other as far as its contribution to the overall composite dielectric behavior.

2)   Mixture responses must be invariant with further random mixing of the type that was employed in order to attain its present state. In other words, if a truly random state has been reached then further 'stirring' does not affect the response of the composite. This property can also be stated as additive functional invariance to mixing by successive stages of mixtures of mixtures. This relation would be

$$f(\epsilon) = \sum_k v_k f(\epsilon_k) \tag{66}$$

where f is a common functional, ϵ is the composite permittivity, ϵ_k is the permittivity of the kth constituent species occupying a volume fraction v_k, and the summation $\sum_k$ is over the k species. This property assumes that constituent volume densities are not affected by successive mixing stages.

3)   The macroscopic dielectric response must be independent of the sample size considered. This results in the mixture response being dependent on relative volume fractions and not overall macroscopic size.

4)   The constituent volume densities must remain constant during the mixing process. This requirement results in the additive relation

$$v_k = \sum_j V_j v_{j,k} \tag{67}$$

where v_k is the fractional volume of the kth constituent species in the present stage of macroscopic volume consideration, V_j is the volume fraction of a submacroscopic volume that goes into the

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present macroscopic volume, and $v_{j,k}$ is the subvolume fraction of the kth species within the jth submacroscopic volume. The summation is exhaustive of all possible j^{th} submacroscopic volume fractions. Presumably, the constituents cannot interact with each other so as to affect the volume density of the other.

The Lichtenecker mixing formula is a self-similarity formula of the type found in references [35-38], meaning that regardless of the macroscopic size scale chosen for observation, one can expect the same result over and over again. In actuality, natural materials may only partially fulfill these requirements, especially if the random mixing occurs only at a particular size scale. Such a violation is evident when considering molecularly interdispersed mixtures, even when otherwise perfectly randomly distributed with no overall sequential ordering.

The exponential averaging factor α of the Lichtenecker mixing formula must be real valued if the mixture is to be causal and obey the complex conjugation property as given by equations (62) and (63). The exact value of the exponential averaging factor α has not been entirely ascertained for random mixtures. The value of the exponential averaging factor must lie within a set of physical bounds called the Wiener bounds. These bounds require that the exponential averaging factor must be real valued at or between minus/plus unity. The value of the exponential averaging factor that is found in a given random composite configuration will depend on spatial degrees of freedom and percolation path(s) available to the displacement fluxes or currents as they traverse the assortment of domain regions. If the composite is built up from submixtures all of the same exponential averaging factor then the composite has the same exponential averaging factor. This then implies the exponential averaging factor has a constant value for a particular mixture type. When the permittivities of the constituents are close to each other then the exponential averaging factor α takes on limiting values which tend to some of the depolarization values which are discussed next.

II) The effective-medium-theory coherent-potential-approximation (EMT-CPA) has been derived and rederived many times [13-15, 39-42]. This approximation is one of the simpler of effective medium theory. Fundamentally, its argument is that a domain region containing one of the constituent permittivities is treated as being surrounded by a medium whose effective permittivity is to be determined. All other domains are treated accordingly with the same approximation of environment. As a further approximation a certain domain geometry is presumed, so as to lend to analytic solution of the electric and displacement fields. The geometry selected is that of ellipsoids, as both Maxwell's electromagnetic equation set can be solved using a conformal coordinate system [16, 17], and because this geometry involves a minimum of structural detail. This treatment corresponds to the lowest order scattering of the solution of Maxwell's electromagnetic equations in an inhomogeneous media

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[15, 43]. This treatment is called the coherent potential approximation. A number of other approximations and refinements can be made using the effective medium technique [32, 44, 45]. However, the approach appropriate to random composites must introduce a minimum of microscopic detail and it is felt the coherent potential approximation does offer such. Further subtreatments do exist in so far as different types of randomness can exist in composites.

An important factor which arises from the effective-medium-theory coherent-potential-approximation (EMT-CPA) approach is the depolarization factor 'A'. The depolarization factor 'A' can be calculated using an integral formula which depends on the ellipsoid shape and is discussed in greater detail in Appendix A [16-18, 32]. In the case of a spheroid situated in N spatial dimensions, the depolarization is simply the inverse of the number of spatial dimensions (degrees of freedom) as

$$A = 1/N .$$
(68)

When constituent permittivities are close valued with respect to each other then the exponential averaging factor can be related to the depolarization as

$$\alpha \to 1 - 2A .$$
(69)

Combining the limit in equation (69) with the identity of equation (68) yields the limiting parameter value

$$\alpha >\to 1-2/N$$
(70)

when the constituent permittivity values are close valued with respect to each other.

In this report we treat both the exponential averaging factor and depolarization as statistical parametric values. Our results are presented on a parametric basis both in terms of the exponential averaging factor 'α' and the depolarization factor 'A' for both clarity of permittivities on relative scales, and presentation of complex numbered permittivities in terms of real valued parameters.

PERCOLATION

The term percolation refers to whether or not there exists a continuous connected path through a constituent species. In the context of the dielectric problem, percolation is whether or not displacement flux/current has at least one path through connected domains of a single constituent species. A permittivity/conductance of zero blocks electric displacement and an infinite permittivity/conductance allows displacement flux/current to pass freely along a path. The situation where the displacement flux/current is in a single constituent but not the other occurs as the limiting case where the permittivities

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are of infinite ratio to one another and there exists a percolation path amongst the larger permittivity domains.

The Weiner bounds (i.e., the series and parallel stratification limits for dielectric composites) can be used to represent the two extremes of percolation behavior. If the constituents lie in flat layers with surface normals oriented parallel to the applied electric field then the exponential averaging factor as defined by equation (1) takes on the value $\alpha = -1$. If the species lie in flat layers with surface normals oriented perpendicular to the electric field then the exponential averaging parameter is $\alpha = +1$. For the depolarization as defined by equation (2), direct substitution of the parameter values $A=1$ and $A=0$ give respectively the series and parallel stratification limits. Thus the depolarization is also a measure of percolation with respect to the Wiener bounds.

Most often percolation is discussed in the context of binary mixtures in which one constituent is nonconducting and the other is fully conducting. It has been found that as the volume fraction of the conducting constituent increases, a transition occurs once a conducting path has been established throughout the composite mixture. This transition is called the percolation threshold. At the percolation threshold, network simulations with iso-sized shuffling elements become self-similar or scaleless [38]. At other constituent mixing ratios this self-similarity may not hold. Lichtenecker's mixture formula stipulates that a self-similarity pattern must always be maintained in a mixture type regardless of constituent mixing ratios. The network simulations used in this report principally employ iso-sized shuffling elements but do not exhibit self-similarity except at percolation thresho..

Percolation mixtures have been extensively studied [38, 46, 47]. It has been found that two-dimensional mixtures with a random sputtering of iso-sized grains have critical percolation transitions at .50 for bond cubic lattices and .59 for site cubic lattices. Our studies of the exponential averaging factor tend to confirm the percolation threshold behavior for conducting/nonconducting binaries. At the percolation threshold the Lichtenecker factor achieves its best self-similarity values.

THE MACROSCOPIC SELECTION

The 'Gaussian' enclosure used in this report is a rectangular box. This choice lends itself to a simple formulation for the macroscopic quantities as well as being easy to envision as a probe parallel-plate capacitor with no fringing fields. The electric field is applied between two opposite faces of the box contacting normally to these surface boundaries. In essence these surfaces form the plates of the probe capacitor. The mean value of the quasistatic electric field is normal to the plate surfaces and has a magnitude of the potential difference divided by the gap distance separating the plates. In numerical

terms this is

$$E = -V/d \qquad (71)$$

where E is the mean electric field magnitude, V is the potential difference, and d is the gap distance separating the plates. The mean value of the displacement field is determined by the displacement flux density averages passing through each of the three opposite face pairs. Thus for each face the mean displacement field can be written as

$$D_n = \Phi/a \qquad (72)$$

where D_n is the magnitude of the mean displacement field component normal to the face, Φ is the displacement flux passing through a face, and 'a' is the surface area of the face. One of the opposite face pairs are the probe capacitor plates. The other two opposite face pairs are termed as lateral faces. The permittivity tensor can be determined using equation (52). The probe capacitor may be oriented along any direction, but for convenience it may be oriented along a principal axis whereupon the electric and displacement fields are colinear. In the isotropic case the displacement and electric field are always colinear which implies that regardless of the orientation there is no lateral displacement flux. We used this fact as a test of isotropy.

The experimentalist may also choose to use a probe capacitance in the comparative sense in isotropic cases. That is

$$\epsilon = \epsilon_o (C/C_o) \qquad (73)$$

where ϵ is the unknown permittivity, ϵ_o is the reference permittivity, C is the measured capacitance with dielectric, and C_o is the reference capacitance.

COMPOSITE DIELECTRIC STRUCTURE

A dielectric composite is a spatial aggregation of interspersed and interconnected permittivity domains. In this report, we seek to calculate the resultant macroscopic permittivity of a composite material for the case of composites which have insignificant quantum overlap between domains. The resultant permittivity can be analyzed in relation to that predicted by the mixture formulae of equations (1) and (2); the results of the numerical simulations will be displayed in terms of the exponential averaging factor 'α' and depolarization factor 'Λ'.

The dielectric composite is solved in terms of a pixel-like rectangular grid as shown in Figure 1. A domain is made up of one or more pixels. Each pixel region is then assigned the permittivity of the domain it represents. Each pixel experiences a local electric field and in turn responds with a displacement

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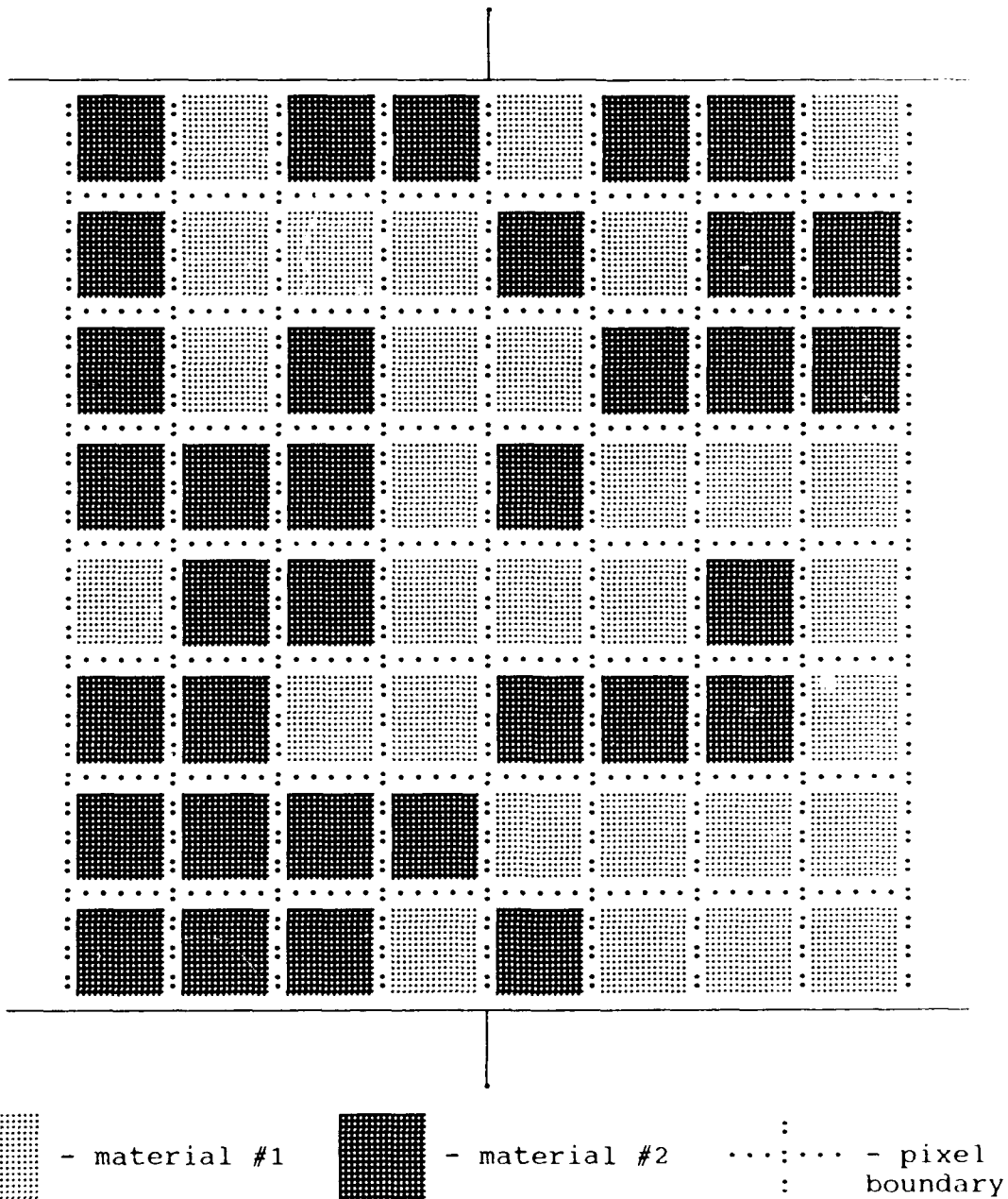
Figure 1. Cross-sectional view of the probe parallel-plate capacitor 'Gaussian' enclosure used in this report. Within the sample region, the composite dielectric is represented by a rectangular pixel arrangement.

field as determined by its assigned permittivity. Displacement field continuity is preserved in passage amongst the pixels. In the general case of a random arrangement of domains there can be strong effects due to local fields when the permittivity

differences are large between the constituents. Even though the macroscopic response tends to wash out local or microscopic details, these small details seem to matter when the mixture is near percolation and the constituent permittivity differences are large. Because of this effect, the numerical analysis requires a fairly high degree of detail or one must somehow cover the crucial details. The approximation employed in this report is a method which is sensitive to at least some degree to local effects.

The pixels are assigned the permittivity value of one of the constituent materials in order not to lend a composite mixing bias to the overall solution, since to assign a pixel a permittivity other than one of the constituent permittivities would require some sort of assumption about possible composite mixing within the pixel region. Such an assumption can only be made once some composite mixture relationship is established.

FINITE DIFFERENCE OR NETWORK ANALYSIS

Equations (10) and (21) may be solved simultaneously and macroscopically to any accuracy using network analysis or equivalently by finite difference approximation. The procedure involves the division of the macroscopic sample into a mesh or node set of macroscopic subregions. By introducing a regular rectangular mesh of points $\{r_i\}$ with spacings δr_{ij} to contacting neighbors one obtains a system of linear equations at each ith mesh point with contacting j^{th} neighbors

$$\sum_j \Phi_{ij} = 0 \qquad (74)$$

or equivalently

$$\sum_j I_{Dij} = 0 \qquad (75)$$

where Φ is the universal displacement flux and $I_D = d\Phi/dt$ is the universal displacement current. The summation is over the jth contacting neighbors of the ith point, and mesh points i and j contain the entire address information needed to specify each mesh point. The displacement flux and current are each determined by the displacement field or displacement current density normal to the interface surface areas surrounding each mesh point. The determination of these quantities is performed as described previously in the discussion of macroscopic dielectric quantities. Expanding equations (74) and (75) one obtains

$$\sum_j D_{ij} \, \delta a_{ij} = 0 \qquad (76)$$

and

$$\sum_j I_{Dij} \, \delta a_{ij} = 0 \qquad (77)$$

where D_{ij} or its time derivative $dD_{Dij}/dt = I_{Dij}$ are respectively

the mean valued displacement field or current normal to surface δa_{ij}, and δa_{ij} is the surface area common to the Gaussian enclosures between the ith and j^{th} nodes. The local displacement field may be related to the local electric field as

$$D_{ij} = \epsilon_{ij} E_{ij} \qquad (78)$$

where D_{ij} and E_{ij} are the mean valued displacement and electric fields on the interface between the ith and j^{th} nodes, and ϵ_{ij} is the permittivity characteristic between the ith and j^{th} nodes. The mean electric field can be expressed quasistatically as a potential difference

$$E_{ij} = \delta V_{ij}/\delta r_{ij} \qquad (79)$$

where E_{ij} is the mean electric field, $\delta V_{ij} = (V_j - V_i)$ is the potential difference between nodes, and $\delta r_{ij} = |r_j - r_i|$ is the internodal separation. The potential or voltage at the ith mesh node point is denoted as V_i. The electric field E_{ij} is the component in the direction perpendicular to the interface shared commonly between the ith and j^{th} nodes. Since rectangular boxes are selected in this report as the type of macroscopic enclosure, the surface normal direction lies along the same direction as the internode gaps δr_{ij} when the nodes are placed at the box centers. Substituting the equations (78) and (79) into equation (76) produces at each ith node the sum over the jth neighbors

$$\sum_j (\epsilon_{ij}\, \delta V_{ij}\, \delta a_{ij})/\delta r_{ij} = 0 \qquad (80)$$

where the notations are as before. The potential drops, $\delta V_{ij} = (V_j - V_i)$, are the unknowns in a system of simultaneous equations formed when all nodes are taken together with an exciting electric field or potential applied across the probe. The factors other than the potential drops in equation (80) may be combined into a set of internodal admittances, yielding

$$\sum_j g_{ij}\, \delta V_{ij} = 0 \qquad (81)$$

with the internodal admittances just $g_{ij} = (\epsilon_{ij}\, \delta a_{ij}/\delta r_{ij})$.

The arguments made in equations (78) through (81) can be repeated in a parallel fashion with the universal displacement current and universal displacement conductivity. One may view this application of Gauss' law as an integral formalism embodied by Kirchoff's rules for a universal displacement current. Each node within the mesh represents a small 'Gaussian' enclosure. The rules of displacement flux/current continuity are then applied to the boundaries between contacting nodes [37, 48, 49].

BOND OR SITE CENTERED PIXEL PERCOLATION APPROXIMATIONS

The generalized path admittance characteristics g_{ij} as given by equation (81) may be assigned on the basis of two pixel percolation approximations as illustrated in Figure 2: 1) site

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        o           ▪           o           ▪           o
        o           ▪           o           ▪           o
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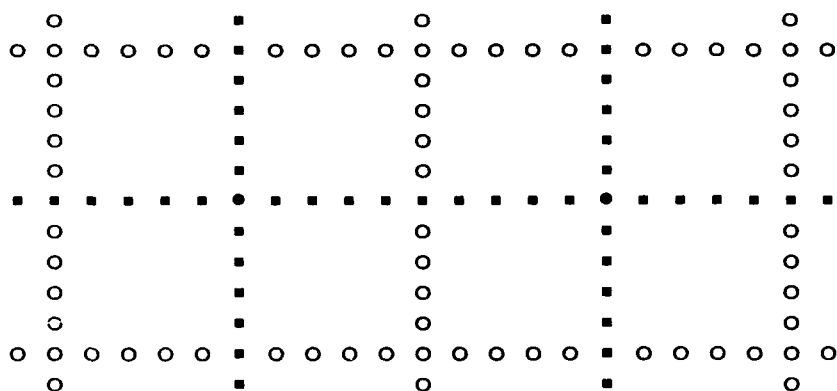
a)   Each path linking adjoining nodes in the site pixel percolation approximation straddles two pixel cell regions. Since a single constituent permittivity is assigned to each pixel, the admittance characteristic of the path is the series combination of the permittivities of both regions.

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  ▪ o ▪                     ▪ o ▪                     ▪ o ▪
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    o       ▪         ▪ o ▪         ▪         ▪ o
    o         ▪     ▪     o     ▪     ▪     ▪     o
    o           ▪ ▪       o       ▪ ▪             o
    o           ●         o         ●             o
    o           ▪ ▪       o       ▪ ▪             o
    o         ▪     ▪     o     ▪     ▪     ▪     o
    o       ▪         ▪ o ▪         ▪         ▪ o
  ▪ o ▪                     ▪ o ▪                     ▪ o ▪
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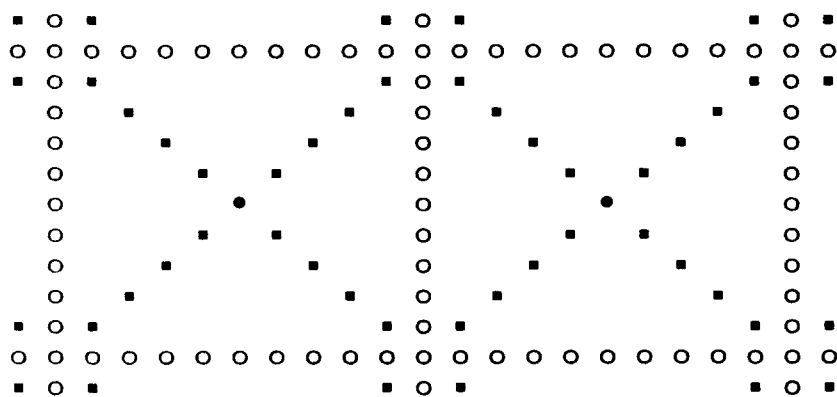
b)   In the bond pixel percolation approximation each displacement flux/current path resides within a single pixel cell region.   The path is assigned the admittance characteristic of the permittivity of the pixel cell.

Figure 2.   Site (a) and bond (b) pixel percolation approximations.   [o o o] designates the pixel cell boundary, [▪ ▪ ▪] outlines a possible displacement flux/current path, and a [●] denotes a node where paths meet.

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centered pixels and 2) bond centered pixels.   In both instances, simulations yield similar trends in the results with some background changes in the overall percolation.

1)   The pixel permittivity/conductivity assignment method in the case of site centered pixels is to assign each mesh node region to a pixel.   In the site representation the internodal paths have two consecutive admittances/conductances which are treated as a

series combination.

2)   The permittivity/conductivity assignments for the case of bond centered pixels are that each internodal path represents a pixel characteristic. Since each pixel has been assigned only one of the constituent characteristics, each path is not a combination of properties.

Both types of arrangements are discussed in the literature on percolation problems [37, 46, 47, 49].

LATERAL BOUNDARY CONDITIONS

The overall rectangular node mesh representing a dielectric composite specimen is solved with exciting electrodes or 'plates' placed in contact with the opposite faces. Continuity of the displacement field requires that the same amount of displacement flux/current which begins on one plate terminates on the other plate. This displacement flux/current boundary condition is satisfied at the plates when the exciting field is solved together with equation (81). This leaves an open question as to how to handle the displacement flux/current on the other (lateral) faces formed by the rectangular mesh that has been superimposed on the dielectric specimen. The displacement flux/current could still enter and exit at the other faces so long as the overall quantity is conserved. As illustrated in Figure 3, two types of lateral boundary conditions are implemented here.

The first and simplest condition is that of 'insulating' faces, wherein we consider the dielectric specimen to be electrically isolated or 'guarded' along the lateral boundaries. In this instance at the lateral boundaries, the normal component of the displacement field approaches zero as no displacement flux can leave the specimen. The 'insulating' boundary condition can be imposed exactly with the computer model although in physical reality this is more difficult to do because of the effect of fringing fields. This condition can be implemented through equation (81) by having the lateral mesh nodes interact only with adjacent interior mesh nodes. The 'insulating' boundary condition is applicable to isolated specimen samples or lattice cells with mirror symmetries and planes.   For example, an ellipsoid has symmetry planes between each pair of semi-axes, and the solution for an octant of the ellipsoid is also the solution for a cubic repeating lattice of ellipsoids with the same repeating symmetry boundaries.

A second type of boundary condition is that of 'periodic' boundaries in which the specimen represents a repeated cell in a cyclic lattice structure. In this case the magnitude of the normal component of the displacement field is the same at similar locations on opposite lateral faces. In some cases either boundary condition can be used on the same problem.

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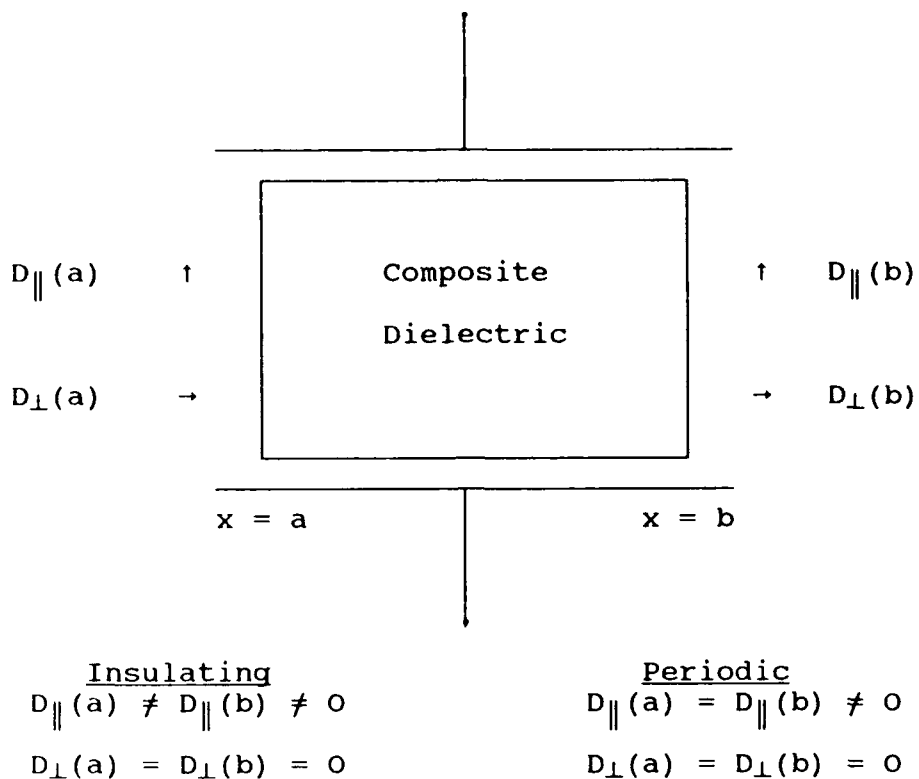
Figure 3. Lateral boundary conditions on the composite dielectric. 'Insulating' means that no displacement flux/current enters or exits the lateral faces. 'Periodic' means that entering or escaping flux/current on a lateral face must enter at a similar location on the opposite lateral face such that overall displacement flux/current conservation is maintained.

In the case of random isotropic media the lateral displacement field becomes a vanishingly small statistical fluctuation and the choice between either set of boundary conditions has little effect on the overall solution. If the distribution of dielectric constituents is not uniformly random but shows an overall anisotropy, a lateral displacement flux/current may occur and the macroscopic permittivity will be nonuniformly tensored.

SOLUTION AND COMPUTER IMPLEMENTATION OF THE NETWORK

The mesh approximation is equivalent to an electrical network or a finite difference grid scheme. The nodes are the intersections between displacement flux/current paths. The electrical elements are the displacement flux/current path admittances between the nodes. The N nodes infer that there are N simultaneous node equations plus one for the exciting node. An important prerequisite to solving this set of N+1 simultaneous

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equations is the choice of a numbering scheme. In the scheme adopted here, the nodes are numbered sequentially from the ground electrode and in relation to (x,y,z) coordinate location. The ith node number is

$$i = x + (y-1)\ X_m + (z-1)\ X_m\ Y_m \tag{82}$$

where (x,y,z) are integers in the range $(1..X_m,\ 1..Y_m,\ 1..Z_m)$. The node address may be specified by the node number i or by the coordinates (x,y,z). The values X_m, Y_m, and Z_m are the extents of the rectangular mesh array in each direction.

The N+1 simultaneous node equations are solved directly and methodically by means of Gauss-Seidal elimination, a plodding but sure fire technique which can be adapted to the mathematics of complex numbers. Back substitution may be invoked to double check the consistency of a numerical solution. By solving the node equations in a sequence that roughly follows the order of the expected node potentials (i.e., the solution is worked from the ground potential up), one can minimize the buildup of truncation errors. The neighbor nodes of the boundary nodes wrap around to the opposite lateral face in the case of periodic or cyclic boundary conditions.

INTERACTION MATRIX

The set of N + 1 mesh equations as formed from equation (81) can be cast into a matrix form. The elements of this matrix are the interactions between nodes. The elements along the main diagonal of the matrix are self-interaction terms corresponding to the sum of all admittance paths connecting to a node. The other elements are the neighbor interactions. When the neighboring node directly adjoins, the corresponding matrix element is the negative admittance of the path. When the nodes are not directly joined by a single bond path, the matrix element is zero. The matrix formalism is convenient because many standard mathematics packages have libraries and function capabilities for matrix operations. The set of equations in matrix form may be written

$$\{\Phi\} = \{g\}\ \{V\} \tag{83}$$

where $\{\Phi\}$ is a column matrix whose elements are the total displacement flux at each node. According to the continuity requirement, all elements of $\{\Phi\}$ are zero except that of the exciting flux. $\{V\}$ is a column matrix whose elements are the node potentials and $\{g\}$ is a matrix representing the admittance interactions between nodes. The admittance matrix $\{g\}$ is symmetric and most off-diagonal elements are zero as they represent interactions between pairs of other than nearest neighbor nodes. (Classical rules of electromagnetism do not allow flux to jump from one region of space to another without an intervening path, thus interactions occur only between adjoining node pairs.) The quantum mechanical formalism does allow for

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nonlocal jumping of displacement flux/current and hence more non-zero terms in the admittance matrix; however, in this report we will only deal with the classical case.

In the sparse symmetric matrix case examined here, a judicious Gauss-Seidal elimination progression proved to be substantially faster than full matrix inversion, especially when the N+1 equations become large. Equation (82) tells us that the maximum node number is the mesh box size which is $N+1 = (X_m Y_m Z_m)+1$. The number of non-zero terms in any row is only the number of neighbors in actual contact. By selecting a node numbering scheme as compact as possible between neighbors it is possible to solve the matrix with a minimum of memory space and computer operation. The solution time for the procedure implemented here went roughly as the square of the admittance interaction matrix size N+1. This allowed simulations of pixels and their mesh networks of up to about 40x40 in two dimensions and 12x12x12 in three dimensions.

The exponential averaging factor 'α' is computed by iteration of equation (1) until a consistent solution is reached between the resultant and constituent permittivities. The depolarization factor 'A' for binary composites can be solved from a quadratic solution of equation (2). The depolarization factor for composites having more than two constituents must be solved iteratively until a self-consistent solution of equation (2) is obtained.

VERIFICATION OF NUMERICAL SOLUTION

The numerical analysis has been implemented using the Hewlett-Packard HP Basic/UX 6.0 programming language, also known as Rocky Mountain Basic. This language follows the IEEE Std 754-1985 for binary numbers. The code is run on an HP 9000 Series 300 workstation with a machine precision of 8 bytes for real numbers and 16 bytes for complex numbers. The precision for complex numbers equates to a precision in the mantissa of about one part in 10^{15}. The accuracy of the numerical solution has been tested in several ways.

The first and most obvious test was the calculation of the macroscopic response of a sequence of layers with surface normals either aligned along or normal to the electric field direction. This could be accomplished by randomizing selectively on successively the $\hat{x}$, $\hat{y}$, and $\hat{z}$ axes. No deviations from the expected limiting Wiener Bounds were found to occur other than truncation errors in the lowest few mantissa bits. A second test was to examine the stability of a given composite layout as it was enlarged or symmetrically folded into another pixel size. Since the physical problem is still the same in the symmetrical sense, then the expected solution cannot vary. The observed results were consistent with our expectations.

We had two methods of matrix inversion available in solving

the nodal analysis. One was the intrinsic matrix inversion built into the HP Basic language and the other was the tailored sparse-advantaged Gauss-Siedal elimination that we developed for the program. The two methods agreed with each other to within machine precision. Furthermore, in either mode the solutions could be checked by back substitution comparison to the original problem. We found errors no worse than in the lowest two or three mantissa bits.

RESULTS

The results of our work are displayed in Figures 4 through 31. Both the exponential averaging factor 'α' and the depolarization factor 'A' are displayed as the volume fraction of the constituents is changed. Both the exponential averaging factor 'α' and the depolarization factor 'A' are real numbers (as opposed to complex numbers) in causal systems, even when the permittivities of the constituents are complex. This fact provides an additional simplification of the results. In Figures 6 through 27, the real part of the averaging factor of interest is denoted with a (+) and the imaginary part with a (-) on the graphs. The imaginary part remains near zero (as expected) and tends to fluctuate markedly less than its real counterpart.

Figures 4 and 5 show respectively the resultant permittivity versus constituent volume for isotropic binary composites of $\epsilon_1 = 1$, $\epsilon_2 = 2$ and $\epsilon_1 = 1$, $\epsilon_2 = 10$. In each case the Wiener bounds are drawn along with several curves at equidistant spacings of exponential averaging and depolarization factors. For the case of nearly equal constituent permittivities as shown in Figure 4, the exponential averaging and depolarization curves are nearly indistinguishable. For larger permittivity differences as shown in Figure 5, the two formulae yield distinctly different results. In these figures, the permittivity is displayed directly to demonstrate that data can be presented in this way, but the curves are squeezed at the ends and lie within a banana-shaped envelope. With complex permittivities of real and lossy parts the data become even more difficult to display. Subsequent figures are thus presented by exponential averaging and depolarization factor windows whose abscissa limits are the Wiener bounds and whose ordinate limits are the minimum and maximum possible constituent volume fractions.

A number of cases are examined and displayed in terms of the exponential averaging and depolarization windows. The first case shown in Figures 6 and 7 is that of three-dimensional spheres spaced in an infinite cubic lattice. For small volume fraction of spheres, this case corresponds correctly to the far field limit of the depolarization expected for dielectric spheres embedded within a host. However, as the volume fraction of the spheres increases, near field changes occur and the depolarization departs from the far field approximation.

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Figures 8 through 27 present various Monte Carlo simulations both in two and three dimensions. The two-dimensional cases in Figures 8 through 13 are complex valued extensions of real-valued analyses from the earlier work [50]. The numerical permittivity simulations have been carried out with both bond and site centered pixel arrangements.

There generally can be a multitude of constituent grain shapes for various heterogeneous composites or mixtures that can be modeled. The simplest possibility is a random shuffling of iso-sized constituent grains. The iso-sized grain case would probably best correspond with molecular mixing without the chemical and quantum interactions. In geology, 'sandy' composites or iso-sized conglomerates could be examples. The iso-sized constituent grain model is mainly what has been approximated by our network models in Figures 8 through 23. Another likely possibility is a composite in which there is a range of constituent grain sizes randomly shuffled. A 'marbled' mixture would have some distribution of assorted constituent grain sizes. Many natural composites exhibit this feature to some degree. Figures 24 through 27 show network simulations where a preliminary effort has been made to include a limited range of constituent grain sizes. Our results indicate an increased scatter which is due to the additional fluctuations induced by having the larger grains present. Also our results still closely approximate the iso-sized case in that the effective medium or depolarization factor 'A' is mostly constant. The calculated values of Lichtenecker's factor 'α' would remain more constant if the same self-similarity pattern were maintained over a composite sample which is much larger than the largest constituent grain. Obviously our network simulations are very limited in this respect. Only near the percolation threshold transition is the self-similarity aspect primarily evident in the grain layout of the iso-sized shuffling case [38]. In the even-numbered Figures 8 through 26 the percolation is approximately marked at the centers of transition in the 'α'-factor.

Indications from the numerical simulations are that both the exponential averaging factor 'α' and the depolarization factor 'A' are nearly congruent for representing the resultant permittivity of composite mixtures where the constituent permittivities differ by less than a factor of two such as in Figures 14 and 15. When the constituent permittivities differ by more than a factor of two, the exponential averaging factor and depolarization factor diverge according to the mixture type. This is evident in the Figures 8 through 13 and 16 through 27. The implication is that the resultant permittivity is dependent on the randomness type involved in the composite, such as whether the constituent grains are iso-sized or have a self-similar range of assorted sizes.

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FAMILY OF PERMITTIVITY CURVES
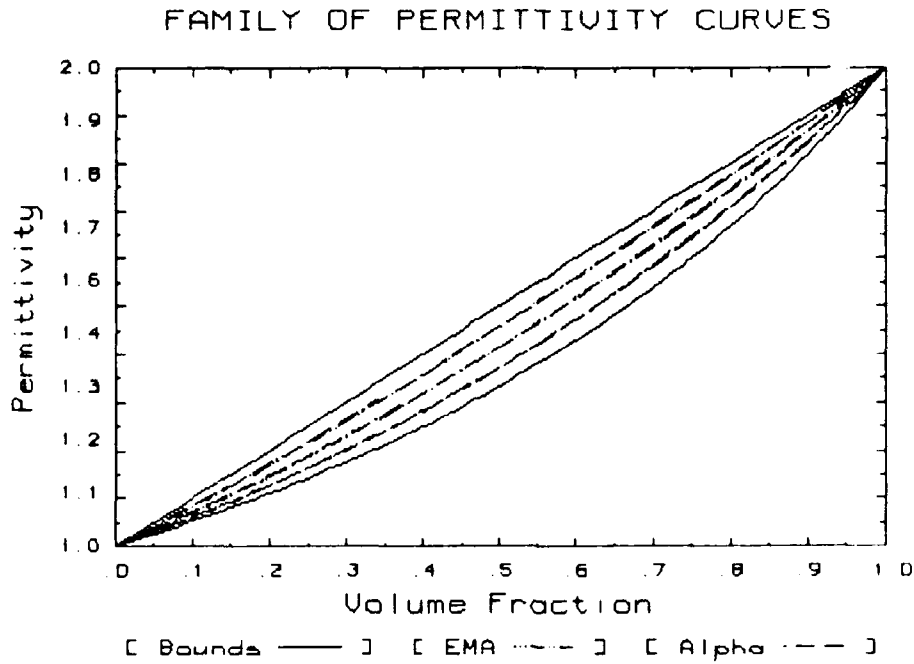
Figure 4. Permittivity curves at ratio $\epsilon_2/\epsilon_1=10$. The curves situated between the Wiener bounds are equally spaced in α and A ranges respectively. ($\alpha=-.50$, A$=.75$, $\alpha=.0$, A$=.50$, $\alpha=.50$, A$=.25$)

FAMILY OF PERMITTIVITY CURVES
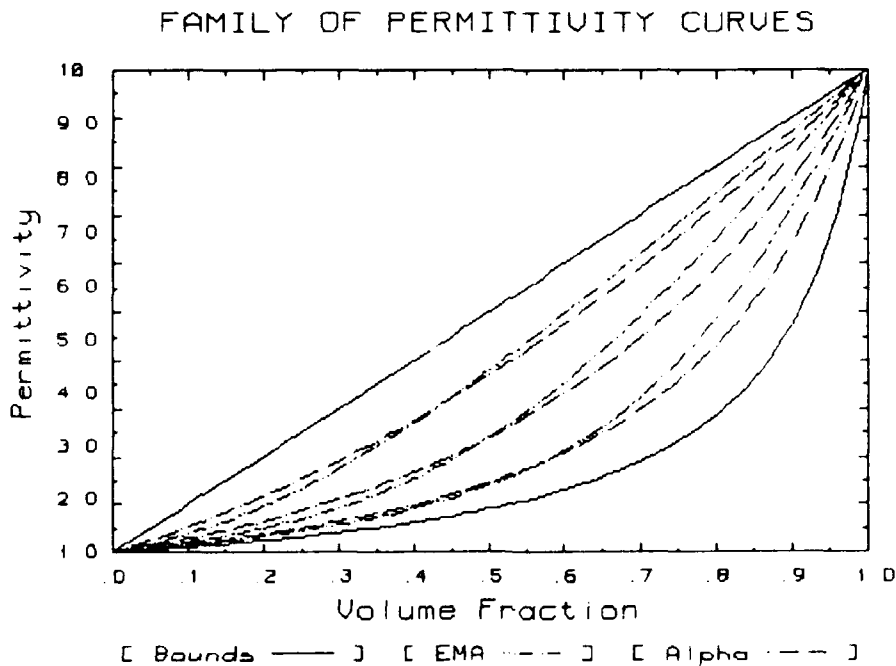
Figure 5. Permittivity curves at ratio $\epsilon_2/\epsilon_1=100$. As above the curves are equally spaced. Note that the bounds envelope expands and each curve pair is less coincident for the larger ratio.

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COMPLEX RANDOM 3D NETWORKS
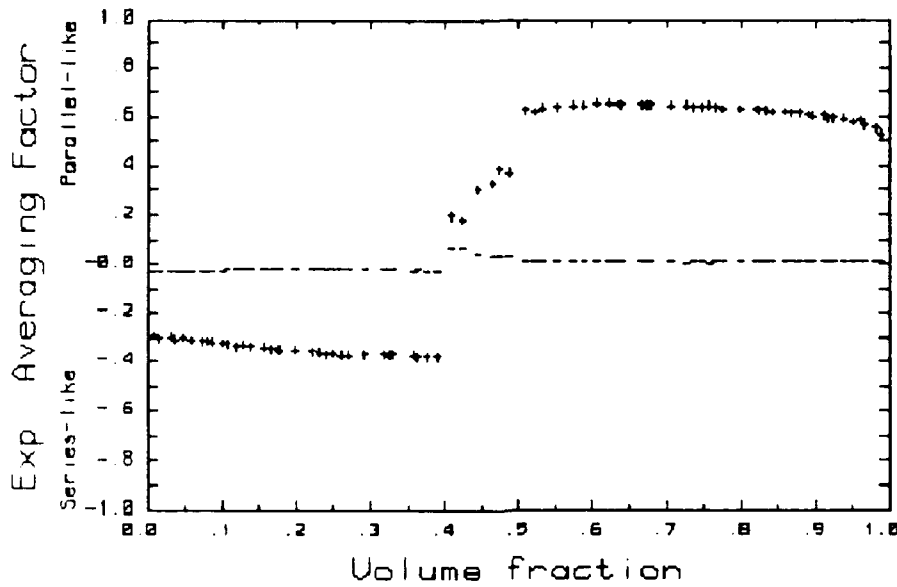
Figure 6. Cubic lattice of spheres with permittivity (1,1000) embedded within a host of permittivity (1,0), α-windowed. Note the percolatic jump which occurs when spheres make contact at closest packing. Resolution 20x20x20 per cell.

COMPLEX RANDOM 3D NETWORKS
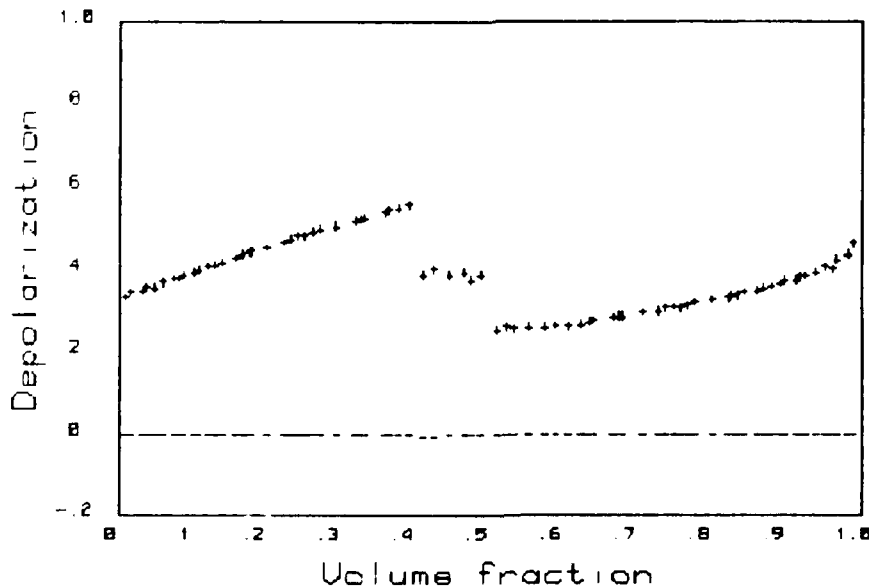
Figure 7. Cubic lattice of spheres with permittivity (1,1000) embedded within a host of permittivity (1,0), A-windowed. The depolarization matches the expected far field limit values at the ends of the volume packing range.

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COMPLEX RANDOM 2D NETWORKS
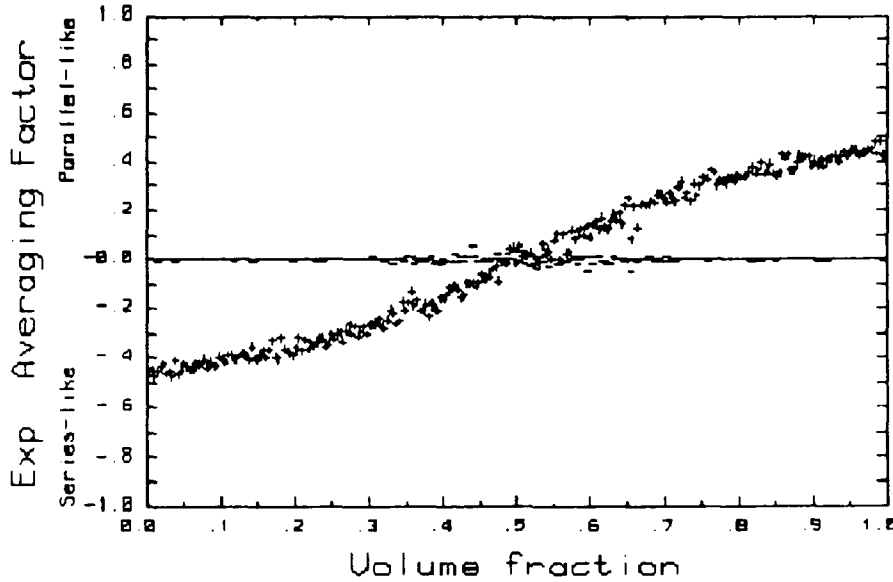
Figure 8. Two-dimensional composite mixture, α-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(0,100)$. Each bond or connecting path is randomly assigned one of the permittivities.

COMPLEX RANDOM 2D NETWORKS
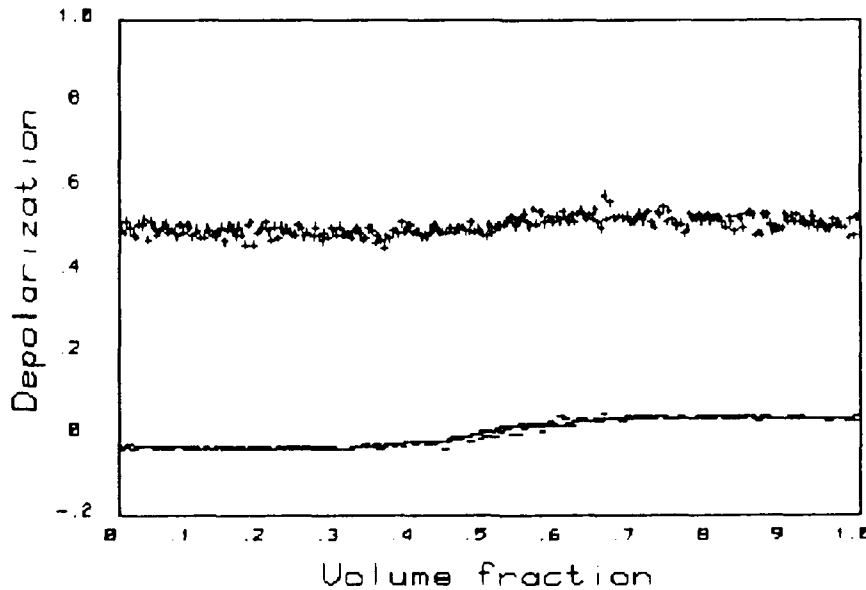
Figure 9. Two-dimensional composite mixture, A-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(0,100)$. Each bond or connecting path is randomly assigned one of the permittivities.

COMPLEX RANDOM 2D NETWORKS
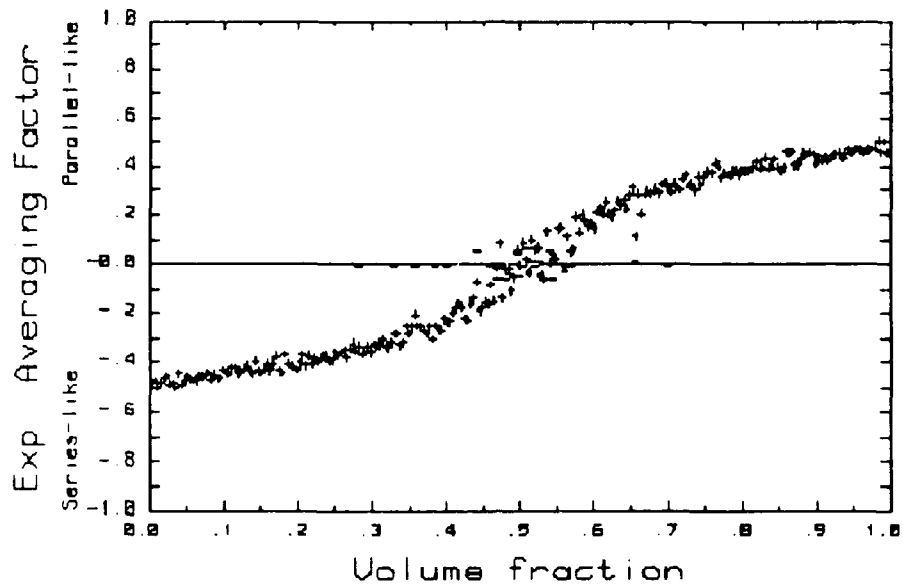
Figure 10. Two-dimensional composite mixture, α-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(0,1000)$. Each bond or connecting path is randomly assigned one of the permittivities. Resolution size at 40x40 bonds.

COMPLEX RANDOM 2D NETWORKS
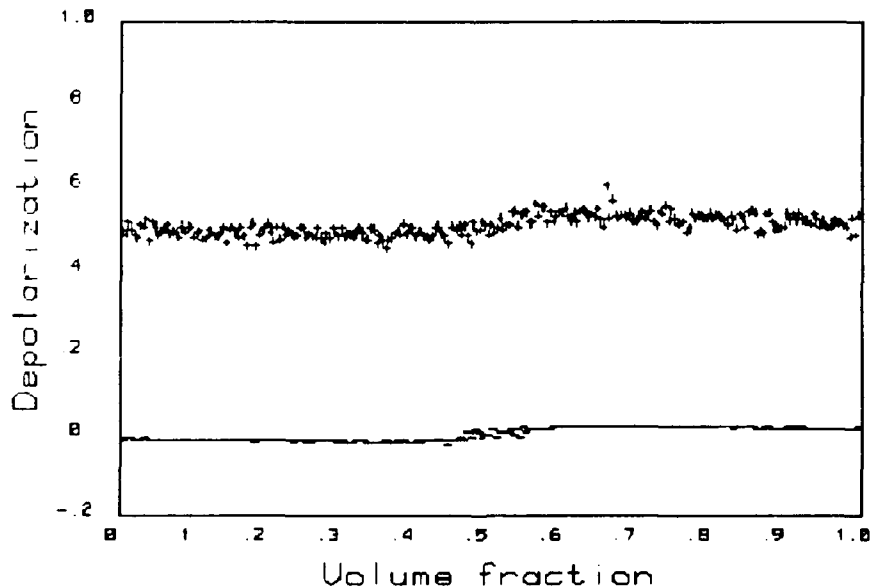
Figure 11. Two-dimensional composite mixture, A-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(0,1000)$. Each bond or connecting path is randomly assigned one of the permittivities.

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COMPLEX RANDOM 2D NETWORKS
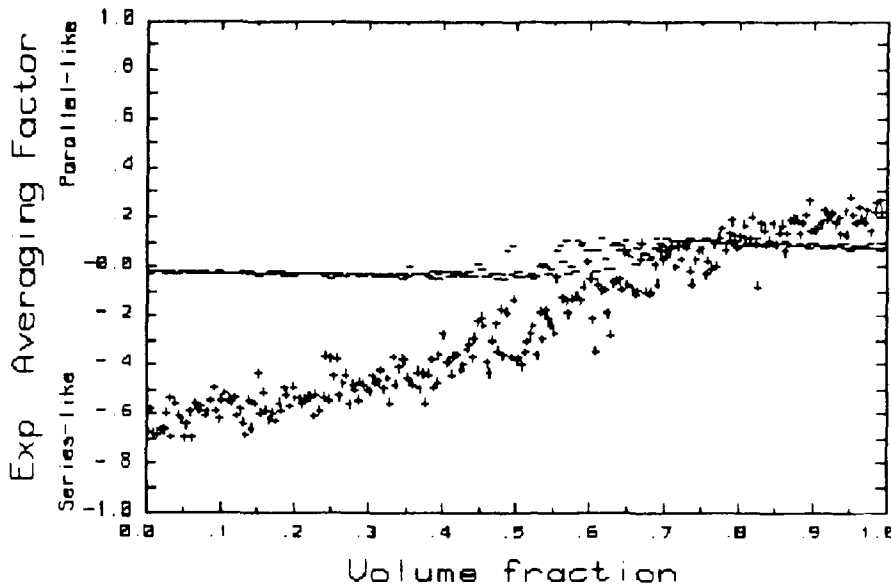
Figure 12. Two-dimensional composite mixture with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(0,100)$, α-windowed. Each site or path cluster surrounding a node is randomly assigned one of the permittivities. Resolution or network size is 20x20 sites.

COMPLEX RANDOM 2D NETWORKS
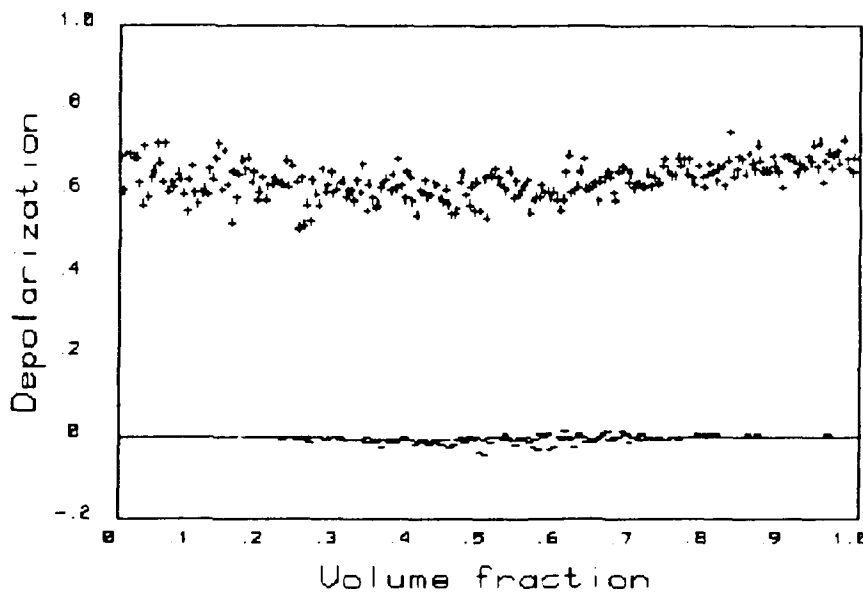
Figure 13. Two-dimensional composite mixture with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(0,100)$, A-windowed. Each bond or node cluster is randomly assigned one of the permittivities.

34
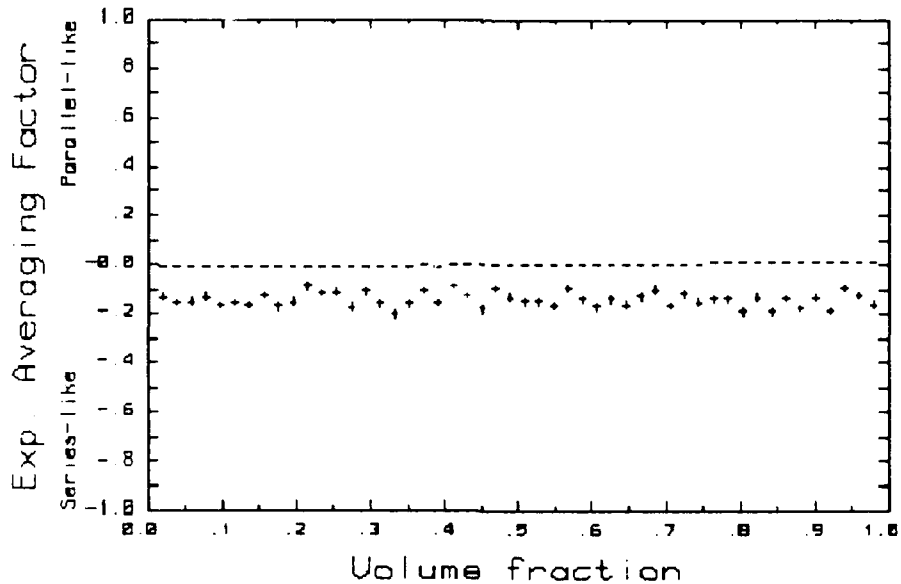
Figure 14.   Three-dimensional composite mixture with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(1,1)$, α-windowed.   Each site or node cluster is randomly assigned one of the permittivities. Resolution size at 10x10x10 bonds.

COMPLEX RANDOM 3D NETWORKS
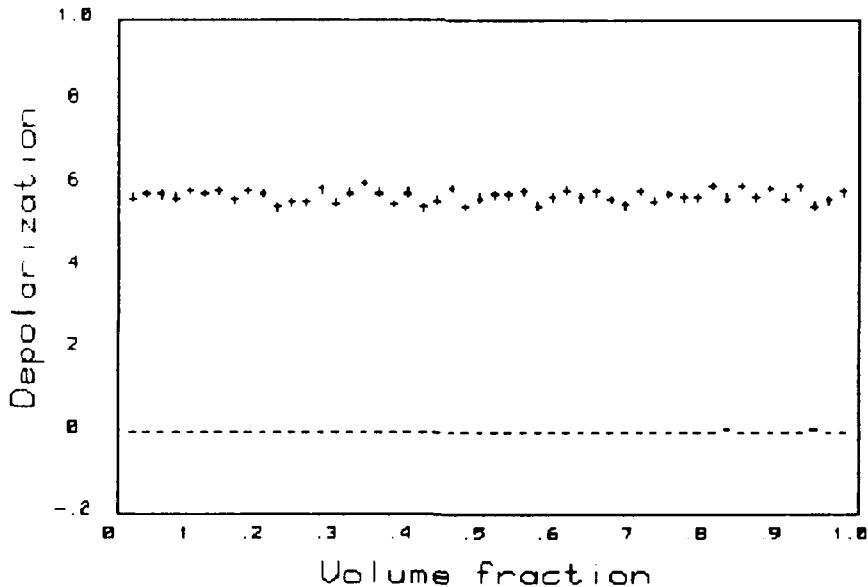
Figure 15.   Three-dimensional composite mixture with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(1,1)$, A-windowed.   Both 'α' and A' curves are nearly coincident in permittivity between the Wiener Bounds.

COMPLEX RANDOM 3D NETWORKS
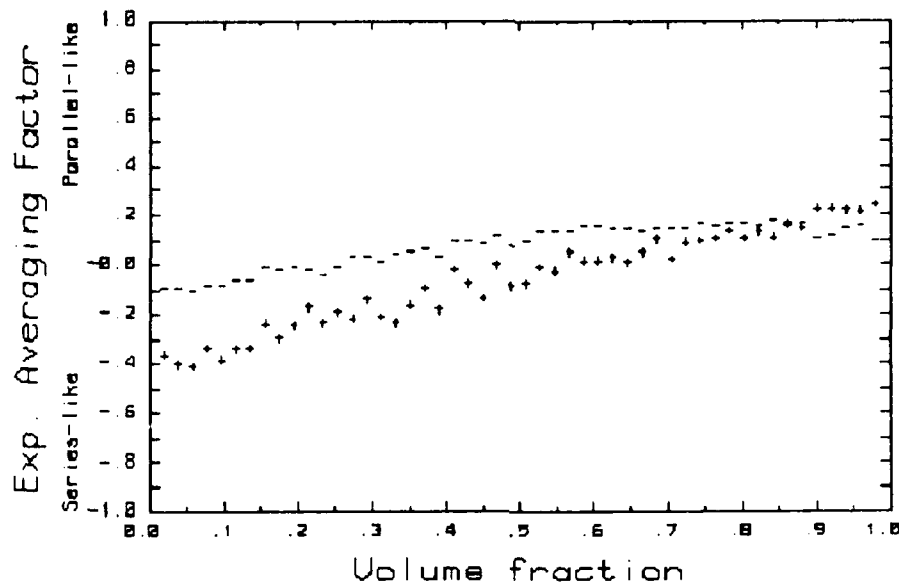
Figure 16. Three-dimensional composite mixture, α-windowed, with constituent permittivities of $\epsilon_1 = (1,0)$ and $\epsilon_2 = (1,10)$ randomly shuffled in a site grid, 10x10x10. Ratio of ϵ_2/ϵ_1 is $(1,10)/(1,0) = (1,10)$.

COMPLEX RANDOM 3D NETWORKS
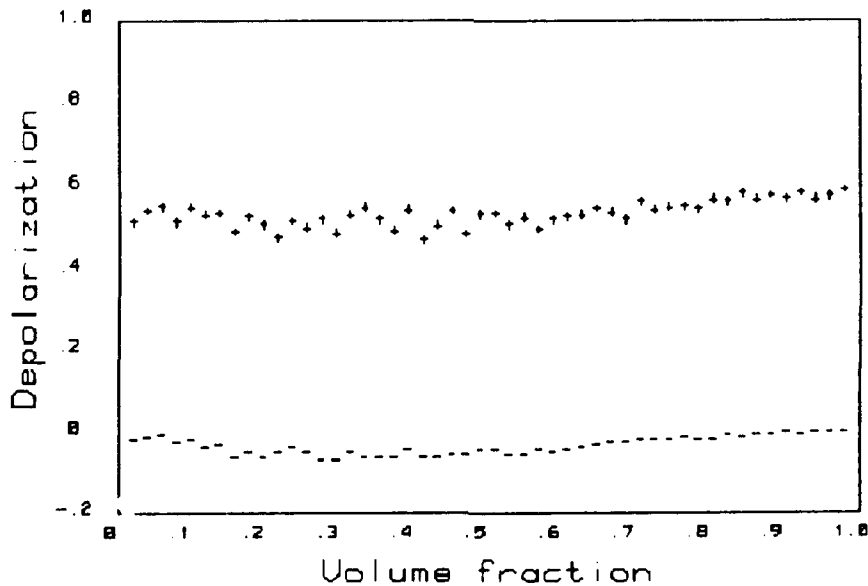
Figure 17. Three-dimensional composite mixture, A-windowed, with constituent permittivities of $\epsilon_1 = (1,0)$ and $\epsilon_2 = (1,10)$ randomly shuffled in a site grid, 10x10x10. Insulated boundary conditions apply. The depolarization remains at about .5.

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COMPLEX RANDOM 3D NETWORKS
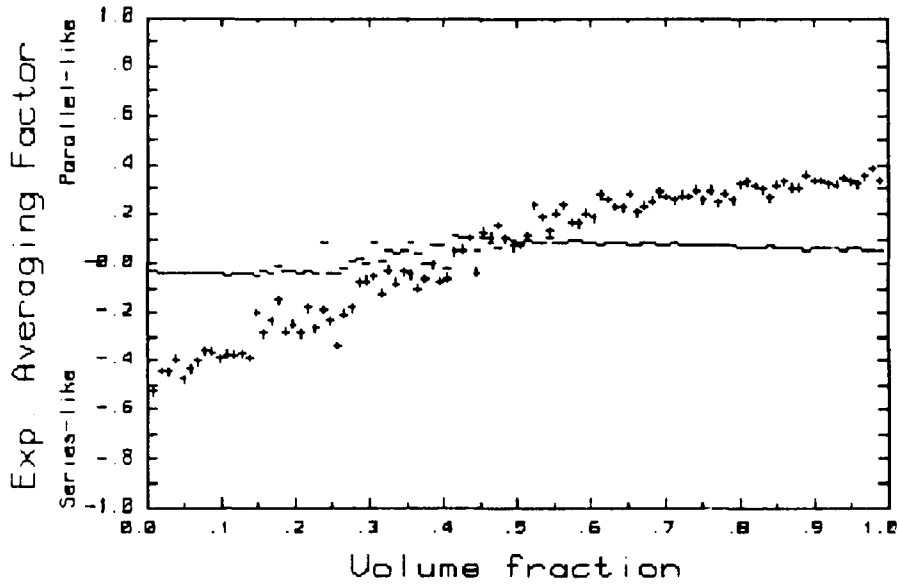
Figure 18. Three-dimensional composite mixture, α-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(1,100)$ randomly shuffled in a site grid, 10x10x10.

COMPLEX RANDOM 3D NETWORKS
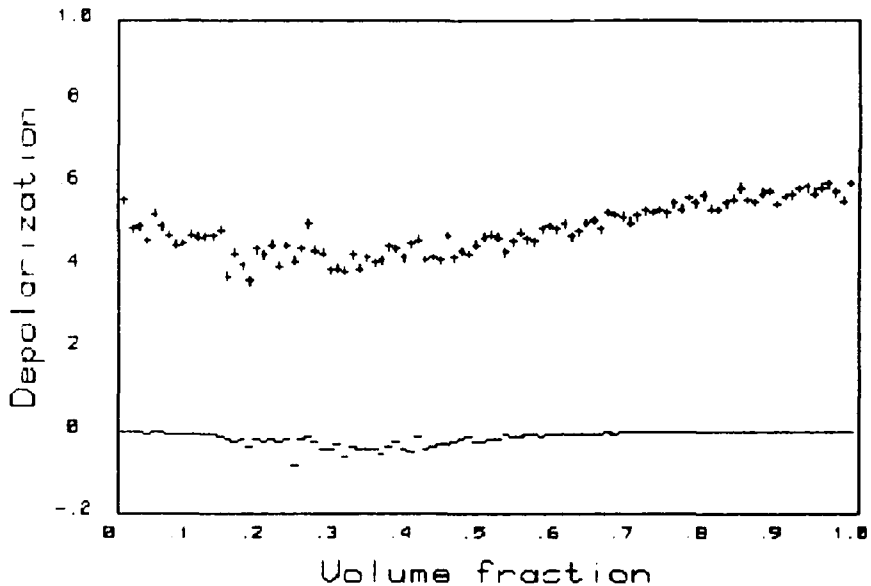
Figure 19. Three-dimensional composite mixture, A-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(1,100)$ randomly shuffled in a site grid, 10x10x10. The depolarization slightly deforms with a minimum around the percolation threshold.

COMPLEX RANDOM 3D NETWORKS
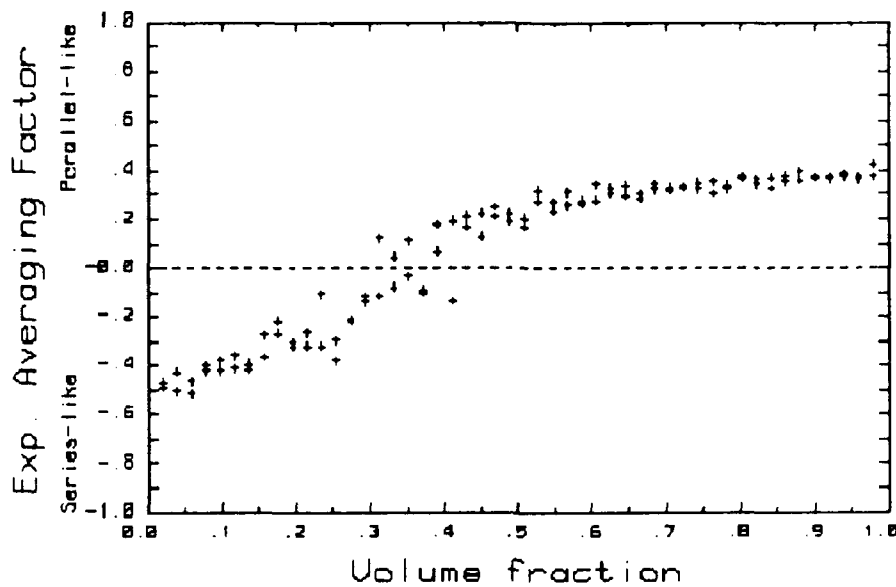
Figure 20.   Three-dimensional composite mixture, α-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(1,1000)$ randomly shuffled in a site grid, 10x10x10.   Insulated lateral boundary conditions apply.

COMPLEX RANDOM 3D NETWORKS
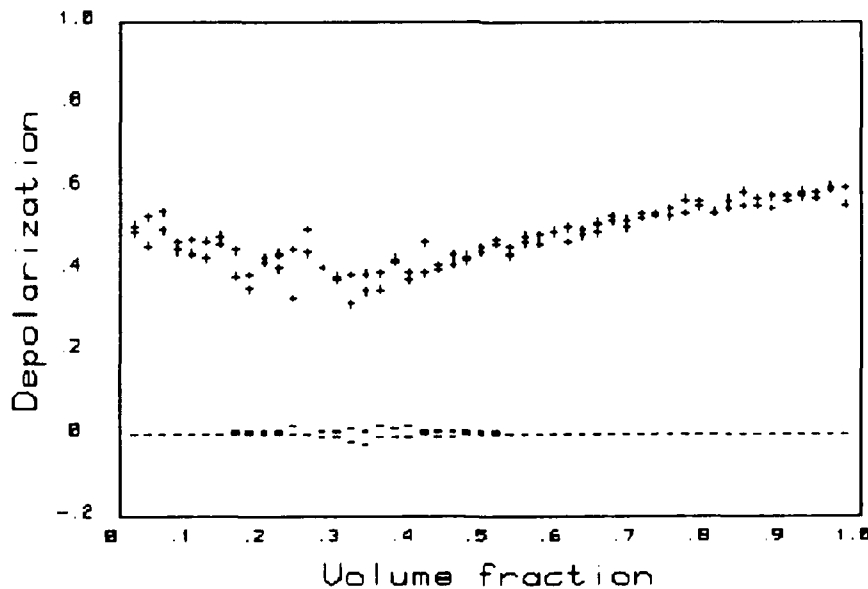
Figure 21.   Three-dimensional composite mixture, A-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(1,1000)$ randomly shuffled in a site grid, 10x10x10.   The depolarization deforms with a minimum around the percolation threshold.

COMPLEX RANDOM 3D NETWORKS
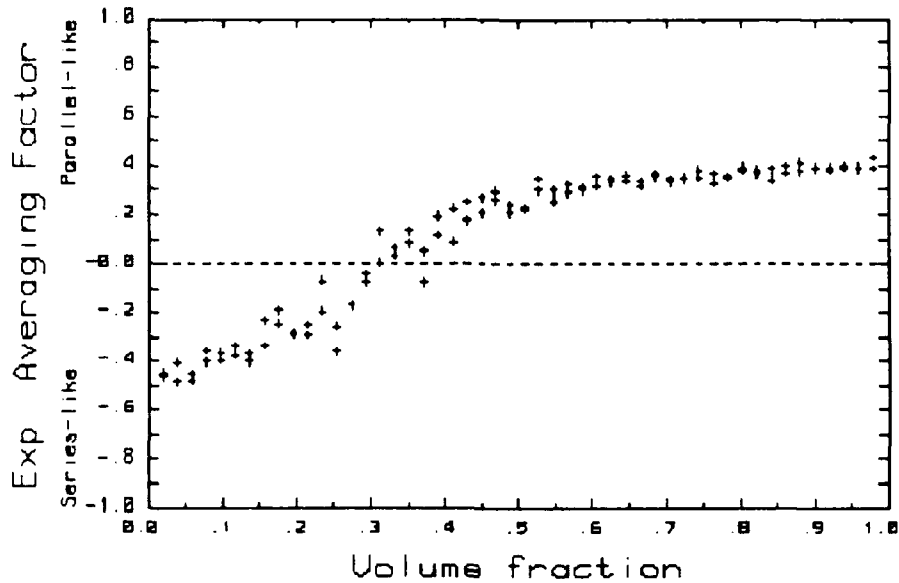
Figure 22. Three-dimensional composite mixture, α-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(1,1000)$ randomly shuffled in a site grid, 10x10x10, with periodic boundary conditions.

COMPLEX RANDOM 3D NETWORKS
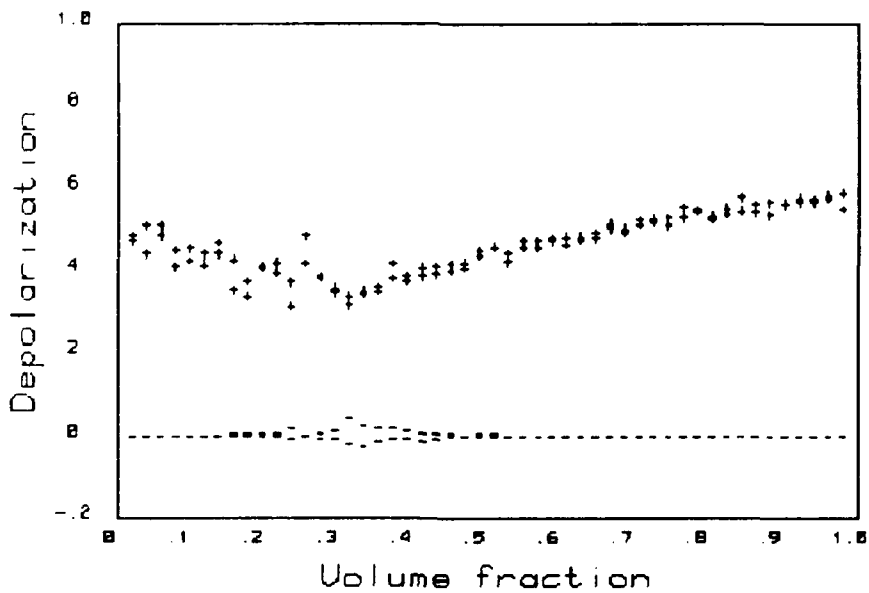
Figure 23. Three-dimensional composite mixture, A-windowed, with constituent permittivities of $\epsilon_1=(1,0)$ and $\epsilon_2=(1,1000)$ randomly shuffled in a site grid, 10x10x10, with periodic boundary conditions. The change from insulated to periodic boundary conditions has little effect on this random case.

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COMPLEX RANDOM 3D NETWORKS
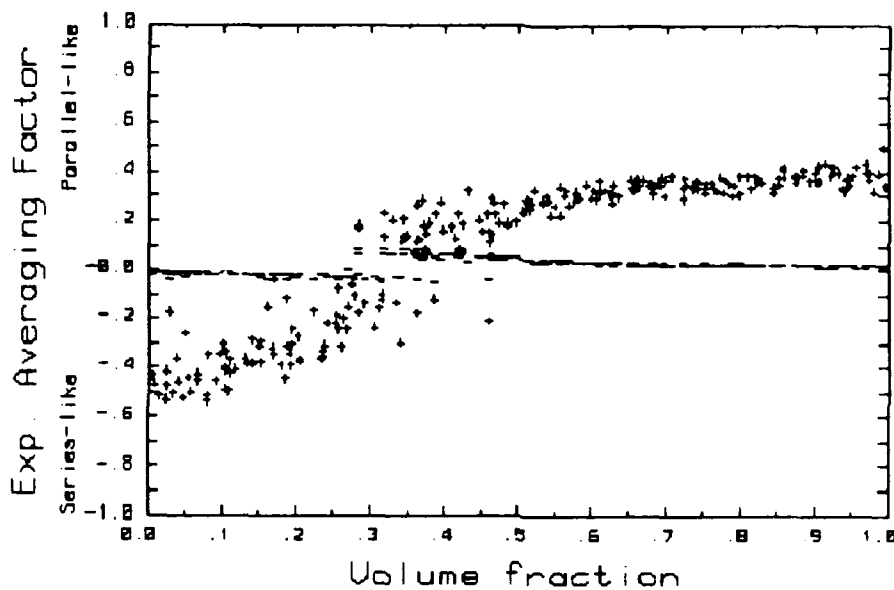
Figure 24.   Three-dimensional composite simulation with 8x8x8 sites, α-windowed, with permittivities $\epsilon_1 = (1,0)$ and $\epsilon_2 = (0,1000)$. Each size stage 2x2x2, 4x4x4, and 8x8x8 is randomly scaled and shuffled.

COMPLEX RANDOM 3D NETWORKS
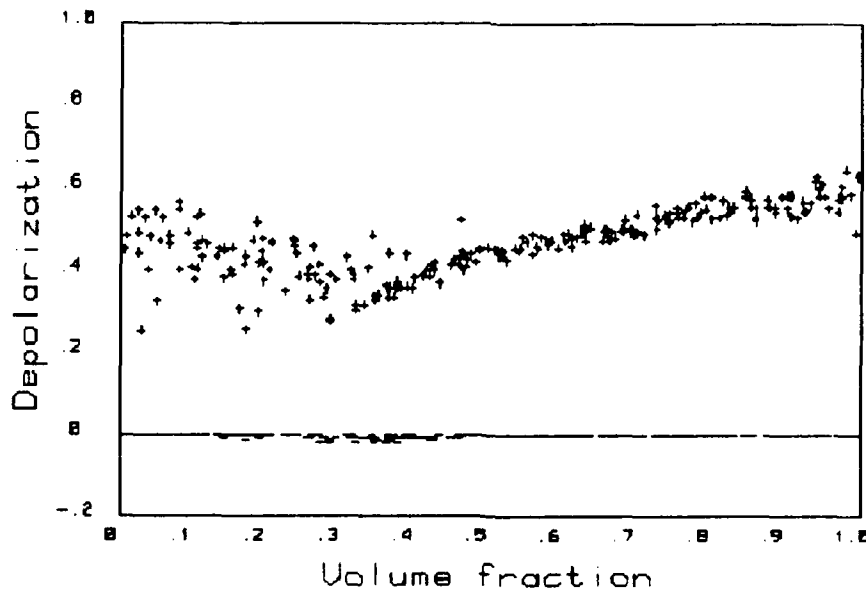
Figure 25.   Three-dimensional composite simulation with 8x8x8 sites, A-windowed, with permittivities $\epsilon_1 = (1,0)$ and $\epsilon_2 = (0,1000)$. Each size stage 2x2x2, 4x4x4, and 8x8x8 is randomly scaled and shuffled. Note that the random composites grains have more scatter as a result of the wider size distribution.

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COMPLEX RANDOM 3D NETWORKS
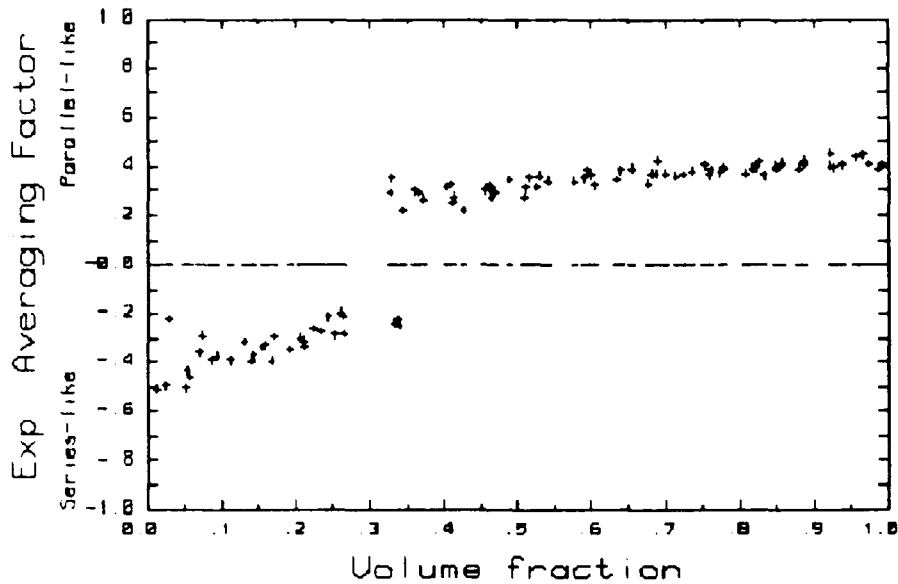
Figure 26.   Three-dimensional composite simulation with 8x8x8 sites, α-windowed, with permittivities $\epsilon_1=(1,0)$ and $\epsilon_2=(0,10^9)$. Each size stage 2x2x2, 4x4x4, and 8x8x8 is randomly scaled and shuffled.

COMPLEX RANDOM 3D NETWORKS
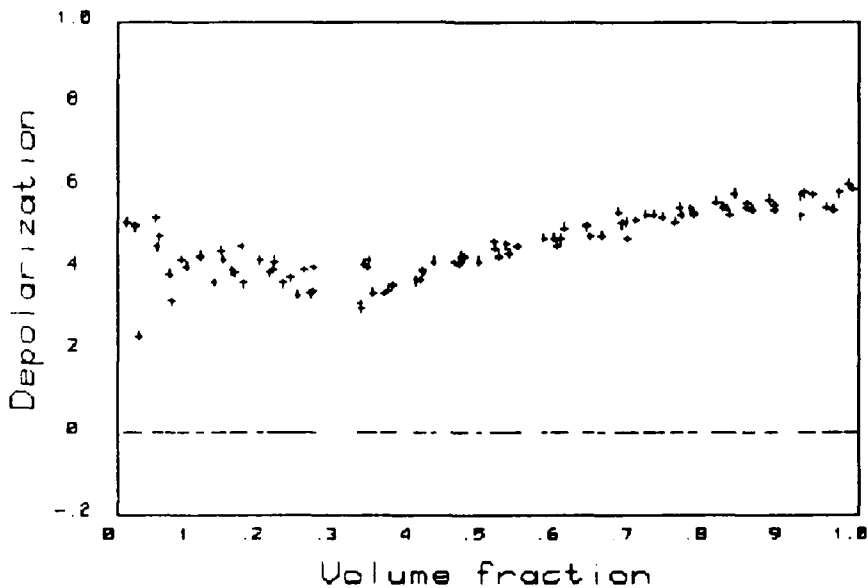
Figure 27.   Three-dimensional composite simulation with 8x8x8 sites, α-windowed, with permittivities $\epsilon_1=(1,0)$ and $\epsilon_2=(0,10^9)$. Each size stage 2x2x2, 4x4x4, and 8x8x8 is randomly scaled and shuffled.   Even at this large ratio of permittivities, back substitution revealed little error.
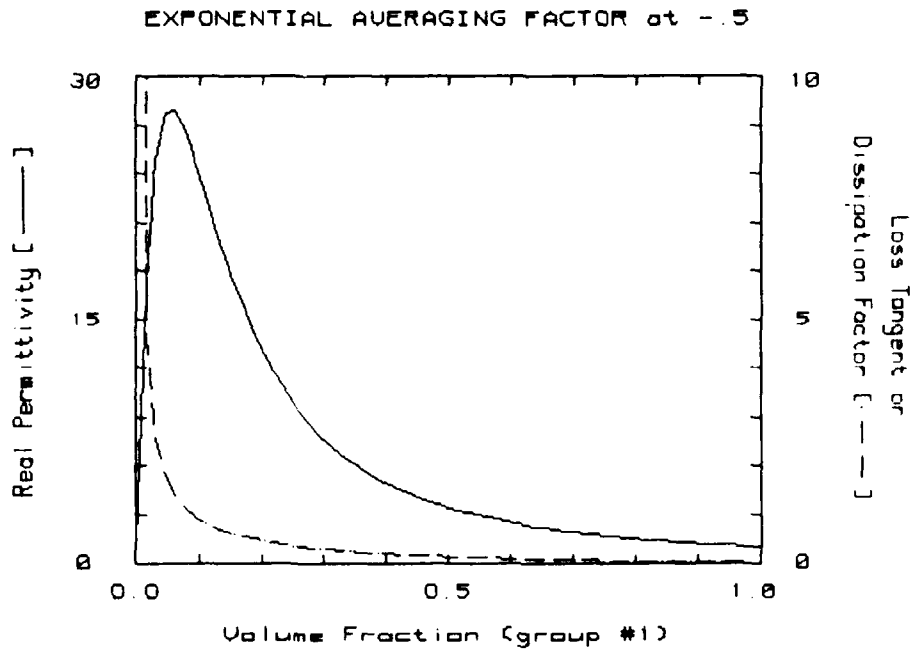
Figure 28.   The Maxwell-Wagner effect of mixing a low loss
constituent with a high loss constituent for permittivities
$\epsilon_1=(1,0)$ and $\epsilon_2=(0,100)$ and $\alpha=-0.5$.
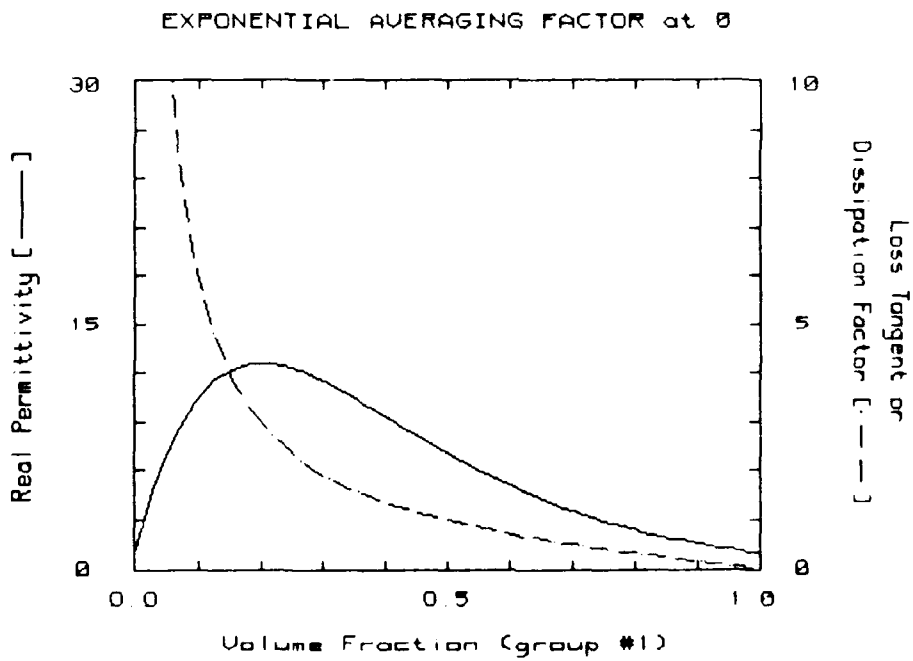
Figure 29.   The Maxwell-Wagner effect of mixing a low loss
constituent with a high loss constituent for permittivities
$\epsilon_i=(1,0)$ and $\epsilon_2=(0,100)$ and $\alpha=0$.
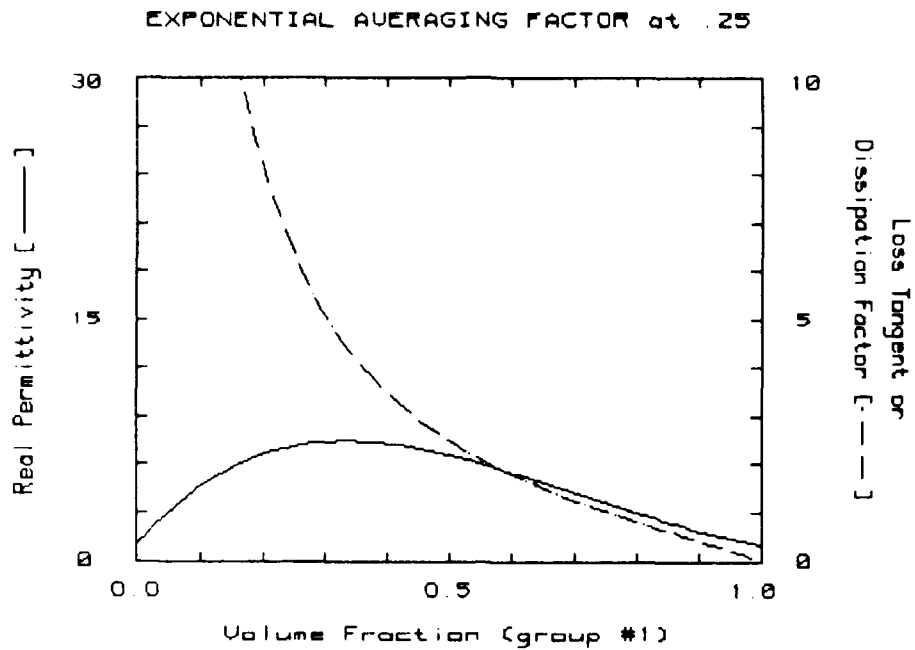
Figure 30.   The Maxwell-Wagner effect of mixing a low loss
constituent with a high loss constituent for permittivities
$\epsilon_1=(1,0)$ and $\epsilon_2=(0,100)$ and $\alpha=0.25$.
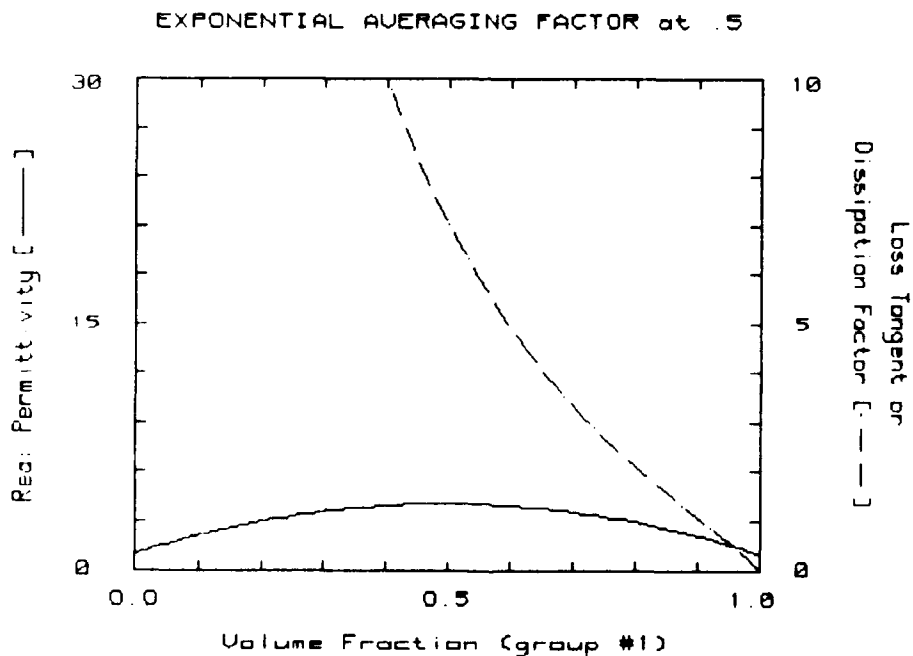
Figure 31.   The Maxwell-Wagner effect of mixing a low loss
constituent with a high loss constituent for permittivities
$\epsilon_1=(1,0)$ and $\epsilon_2=(0,100)$ and $\alpha=0.5$.

LOG-LOG 2D RUN TIMES
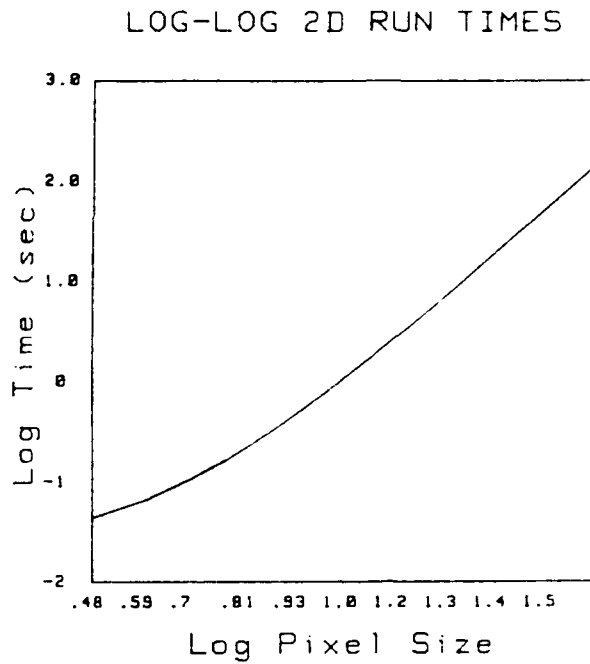
Figure 32.   Run times for two-dimensional simulations.

LOG-LOG 3D RUN TIMES
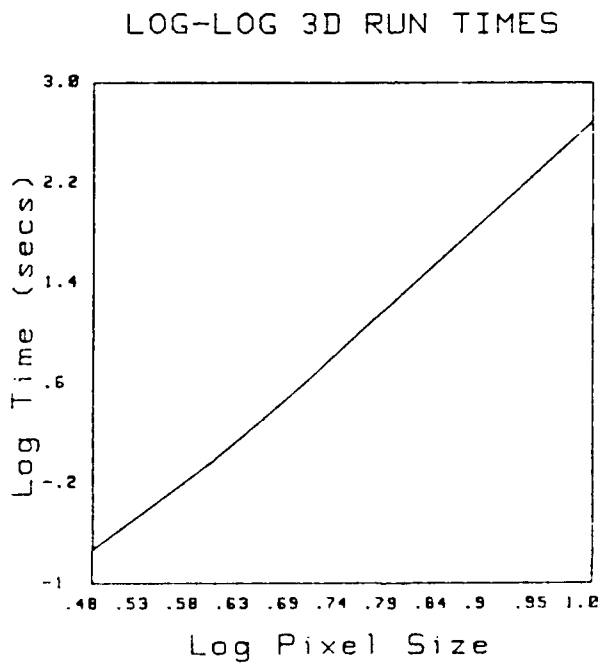
Figure 33.   Run times for three-dimensional simulations.

FUTURE WORK

The completion of the design and computer coding for the bond and site models for composite dielectrics opens up a large range of research possibilities. Future work should include:

a)   Analysis of composites with three or more components. Studies allowing mixture formulae to be employed within the pixels in a fashion self-consistent with the overall composite solution.

b)   Studies of the mapping of the displacement field and the electric field within specimens.

c)   Extension to cases of dyadic or tensorial permittivity constituents and composite dielectric response.

d)   Study of fractal and self-similar composites especially random fractals and scaling of percolation. Fractal dimensionality and spatial correlation layout measurements would reflect the degree of self-similarity and also allow spectral dimensionality considerations.

e)   Investigation of the Maxwell-Wagner effect over different types of composite mixtures.

f)   Development of engineering design code, tables, and approximations which make these composite mixture formulae easily accessible.

g)   Extension to pole-zero analysis and design of artificial dielectrics as well as the utilization of the Kramers-Kronig relations for cross-checking laboratory data as to causality or the interpolation and smoothing of partial data gaps. Examination of the relationship between our network studies and the phenomena of universal type of frequency dependence in ponderable dielectric properties as exhibited by many substances.

h)   Studies of stretched, elongated, and stratified composites.

i)   Studies of quantum overlap, quantum sensitive, and non-local effects.

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APPENDIX A. Depolarization

The resultant permittivity of a dielectric ellipsoid of one permittivity embedded in a medium of another permittivity can be determined by solving Laplace's equation within each of the media using confocal ellipsoidal harmonics [16-18, 30, 31, 51-55]. The solutions for the two regions are then matched at the dielectric interface according to the boundary conditions of continuity of the normal component of the electric displacement field and continuity of the tangential component of the electric field. A geometric factor related to the ellipsoid shape which emerges from the solution is

$$A_p = \frac{abc}{2} \int_0^\infty \frac{du}{R\,(u+p^2)} \qquad (p=a,b,c)$$

where a, b, and c are the ellipsoid axes and A_p is the depolarization factor when the overall fields are aligned along an axis. Accordingly, within the integral p assumes the value of a, b, or c.   The function R is defined by positive R^2 = $(x+a^2)(x+b^2)(x+c^2)$.   Integration by parts yields the identity $A_a+A_b+A_c = 1$.   Thus the relation for the case a=b=c is A =1/3. The two-dimensional case is obtained by examining the limit as one of the ellipse axes goes to infinity so as to effectively eliminate it from the integral. Thus in the two-dimensional case the identity is A_a+A_b = 1 *and for* a=b we have A = 1/2. The same procedure can be applied to solve the one-dimensional case giving the trivial solution of A = 1.   In general, a spheroid (ellipsoid with a=b=c) has a depolarization of A = 1/N, where N is the number of spatial dimensions. Other oblate and prolate cases can also be evaluated directly with the depolarization integral.

APPENDIX B.   Program Codes

```
     _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _
                                "DIEL_BOND"
          Program in HP BASIC for numeric analysis based on the bond model
     _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _

10    !  <  <  <  <  <  <  < "DIEL_BONDS"  >  >  >  >  >  >  >
20    ! * - * - * - * - * - * - * - * - * - * - * - * - * - * - * - * - *
30    !  A main program to evaluate a 3 dimensional composite complex
40    !  dielectric response for a pixel network of capacitors.
50    !                                              S. R. Wallin, 6/1/91
60    ! * - * - * - * - * - * - * - * - * - * - * - * - * - * - * - * - *
70    PRINT " MEMORY IS";VAL(SYSTEM$("AVAILABLE MEMORY"))/8;"(reals)"
80    OPTION BASE 1
90    DATA 1,0,2,1,4,3,7,6,11,10,16,15,22,21,29,28,37,36 ! Prog diel data
100   COM /Pass/Relay(0:7)                     ! for sharing to subs 1 var
110   COM /Pixel/Chdr$[80],Dhdr$[80],INTEGER Lxtnt,Pixl(1:20,1:20,1:20)
120   COMPLEX Hpiv(1:202),Hpr(1:10000)    ! dim to reasonable size for 3D
130   DIM Hdr$[80]                         ! available string for headers
140   COMPLEX Admt(0:7),Adms1,Adms2        ! neighbor admittance values
150   INTEGER Kube,Xt(0:7),Yt(0:7),Zt(0:7)  ! neighbor addresses
160   COM /Memr/Graf(1:512,1:4),Ahdr$[80],Bhdr$[80],INTEGER Rep,Kwd  !trials mem
170   !***> COM areas can be reaccessed with next RUN if identical name & sizes
180   !***> nb., max Lside >= .5 + cube root(.25 + 2*(max dim - 1) )
190   LET Start=TIMEDATE
200   INTEGER Lside,Kond,Nodesz
210   INTEGER Ptrn,Nd,Nd1,Nd2,Boxes,Slant,Sprss
220   INTEGER Xkin,Ykin,Zkin,Xcnt,Ycnt,Zcnt,Xaddr,Yaddr,Zaddr
230   INTEGER Qdrnt,Rptr,Trans,Pose,Grpt,Tls,Sctr,Itmp,Occp,Nsvf,Rsw
240   INTEGER Hmem,Hedge,Hpremax,Hopped,Hsteps,Hnde,Hcnt,Kcnt,Hkm
250   INTEGER Cnmb,Hnbr(0:7),Hcnr,Jxt
260   DIM Frpx(0:9),Msd$[60],Fln$[60],Fsv$[60]
270   COMPLEX Ctmp,Resp,Hnrm,Diel(1:9)
280   LET Grpt=0                          ! Initialize the data storage counter
290   ! * - * - * - * - * - * - * - * - * - * - * - * - * - * - * - * - *
300   !    for which the integer variables roles are:
310   !    Relay = an available common pass variables
320   !    Lside = the # of pixel capacitor elements encounter along an edge
330   !             of the square of pixels
340   !    Tls = Lside or Lside/2 if 2x2x2 tiling
350   !    Qdrnt =  quadrant pixel array expanding switch, 0=off & 1=on
360   !    Px_tot = total # of pixels in square = Lside*Lside
370   !    Rsw = even/odd switch, etc
380   !    Kond = the boundary condition on the sides of the overall composite
390   !            capacitor, 1) insulating sides or 2) periodic or sides which
400   !            wrap around
410   !    Nodesz = the maximum number of interaction nodes in forming
420   !            network, with 0 as the ground or base plate, 1 as center
430   !            node, and the final node number for the top plate.
440   !            Its value is: L*L*L/4+L*L/4-5L/2+4
450   !
460   !                X SECTION OF CAPACITOR CUBE
470   !                                   |
```

```
480  !                               |
490  !                    ===================== top node or plate
500  !                     X X X X X X X X X
510  !                     X X X X X X X X X
520  !                     X X X X X X X X X
530  !                     X X X X X X X X X
540  !                     X X X X X X X X X  center node at midpoint
550  !                     X X X X X X X X X
560  !                     X X X X X X X X X
570  !                     X X X X X X X X X
580  !                     X X X X X X X X X
590  !                    ===================== base node or plate
600  !                          _|_
610  !
620  !                           __       ...  X's represent nodes
6 )  !                          _
640  !     Pixl() = the overlaying matrix representing the capacitor pixels
650  !     Dsplc() = displacement current of pixel per normalized volt/meter
660  !     Potnt() = pixel voltage relative to one volt across entire sample
670  !     Diel() = dielectric value or admittance value of a capacitor pixel
680  !             attached to addresses represented in the pixel grid
690  !     Frpx() = volume fractions associated with pixel types
700  !     Xt(),Yt() = neighbor addresses
710  !     Fln$ = string refering to a filename, Hdr$ = 80 chars
720  !     Ahdr$,Bhdr$ = headers of 80 chrs for Data Title & ID for COM /Memr/
730  !     Chdr$,Dhdr$ = headers of 80 chrs for Pixel Title & ID for COM /Pixel/
740  !     Ptrn = choice of pixel grid filling pattern
750  !     Nd = a single number label for a node
760  !     Nd1,Nd2 = refers to a 1st node & a 2nd node @ specified by single
770  !             node numbers
780  !     Xkin,Ykin,Zkin = kinship 3D address of a node number ie (x,y,z)
790  !     Xcnt,Ycnt,Zcnt = step counters to pixels neighbouring a node in 3D
800  !     Xaddr,Yaddr,Zaddr = addresses of neighbouring pixels in 3D
810  !     Boxes = total concentric boxes fitting within pixel grid or
820  !             number of 2x2 cell blocks along an edge on pixel grid
830  !     Jxt = a juxtaposition counter
840  !     Kube = inside cube territory test
850  !     Slant = 0 if foward slash or 1 if backslash slanting capacitor
860  !     Rep,Rptr = overall number of repeats, Kwd=# of data storage types
870  !     Grpt = overall plus transpose repeats for use of data storage
880  !     Sprss = Suppression of printout details
890  !     Trans,Pose = Pixel transpose selection
900  !     Resp = Overall dielectric response of pixel sample along E
910  !     Nsvf = switch indicating if intended to save repeat info
920  !     Tmp,Tmp1,Tmp2,Vt1,Vt2 = reals available for various uses
930  ! * - * - * - * - * - * - * - *   * - * - * - * - * - * - * - * - *
940  PRINT
950  PRINT " > > > Happy capacitor composite adventures in 3 dimensions < < <"
960  PRINT "                  preformed on ";DATE$(TIMEDATE);
970  PRINT " at ";TIME$(TIMEDATE)
980  PRINT
990  ! #  #  #  #  #  #  #  #  #  #  #  #  #  #  #  #  #  #
1000 ! The hopper reduction subarray:              S. Wallin, July 1990
1010 !       ____  .  .  .  .  .  .  .  .  > large symmetric sparse matrix .
1020 !     | 1,1|    <=< NODE PAIR
```

```
1030  !       |_#1_|____  <=<hopper address                          .
1040  !       | 2,1| 2,2|                                            .
1050  !       |_#2_|_#3_|____                                        .
1060  !       | 3,1| 3,2| 3,3|                                       .
1070  !       |_#4_|_#5_|_#6_|                                       .
1080  !    .                ..        The hopper subarray moves       .
1090  !    .                       .. down as pivoting progresses     .
11C0  !   \/ lg sym sparse matrix        ..                          .
1110  !   . . . . . . . . . . . . . . . . . . . . . . . .
1120  ! The "H" prefix is mainly used to denote variable use in hopper program
1130  ! Hnbr(*) = neighbor nodes
1140  ! Hedge = altitude or base or diag # elements of reduction hopper
1150  ! Hmem = the total # of elements contained within reduction hopper
1160  ! Hpremax = same as Hmem but less Hedge (ie less largest row)
1170  ! Hsteps = extent of larger interaction matrix upon hopper reduces
1180  ! Hcnr = corner node #s of insulated sides Pixel grid cube
1190  ! Hpiv() = Pivoting vector of node reduction
1200  ! Hpr() = working hopper array of matrix reduction
1210  ! # # # # # # # # # # # # # # # # # #
1220  PRINT ">Try hopping along to a solution of sparse matrices at ";
1230  DISP "IO to be: 0)default 1)lab 3.5"" 2)lab hardisc 3,4)A,B office ";
1240  INPUT "5)user defined",Nd
1250  IF Nd<0 THEN STOP
1260  IF Nd=0 THEN Msd$=""
1270  IF Nd=1 THEN Msd$=":CS80,700,1"
1280  IF Nd=2 THEN Msd$=":CS80,700"
1290  IF Nd=3 THEN Msd$=":CS80,703,0"
1300  IF Nd=4 THEN Msd$=":CS80,703,1"
1310  IF Nd=5 THEN INPUT "Name (completely) storage?",Msd$
1320  IF Msd$<>"" THEN PRINT RPT$(" ",50);"storage";Msd$
1330  PRINT " The pattern choices are:"
1340  PRINT "  0) internal, via COM /Memr/"
1350  PRINT "  1) from file storage"
1360  PRINT "  2) every pixel filled by user"
1370  PRINT "  3) random (i.e. well mixed)"
1380  PRINT "  4) by slanted fill level"
1390  PRINT "  5) with  an circle or ellipse of which can be tilted"
1400  PRINT "  6) with strata"
1410  PRINT "  7) concentric boxes"
1420  PRINT "  8) an ellipse with host & inclusion (2 components only,";
1430  PRINT " but symm wrt 1/2 vol)"
1440  INPUT "Select design of pixel grid? (see above)",Ptrn
1450  IF Ptrn<0 THEN STOP
1460  !DISP " & boundary conditions? 1) Insulative ";
1470  !INPUT "2) Wrap around or periodic",Kond
1480  LET Kond=1 !TEMPORARY
1490  IF Kond<0 THEN STOP
1500  IF Kond=0 THEN Kond=1
1510  IF Kond>2 THEN Kond=1+BIT(Kond+1,0)
1520  !INPUT "Use 2x2x2 tiles on pixel grid? 0) No 1) Yes",Tls
1530  Tls=0 !temporary until programmed
1540  IF Tls<0 THEN STOP
1550  LET Tls=1+(Tls=1)
1560  !INPUT "Oct- fold symmetry expansion of pixel grid? 0) No 1) Yes",Qdrnt
1570  LET Qdrnt=0 !temporary until programmed
```

```
1580   IF Qdrnt<0 THEN STOP
1590   LET Qdrnt=1+(Qdrnt=1)
1600   SELECT Ptrn
1610   CASE =0
1620     IF Lxtnt<2 THEN
1630       PRINT " Are Pixels there in memory? ..idled ..start again"
1640       STOP
1650     END IF
1660     IF Lxtnt>21 THEN PRINT " .. there may be too many Pixels"
1670     REDIM Pixl(1:Lxtnt,1:Lxtnt,1:Lxtnt)
1680     LET Lside=Lxtnt*Qdrnt*Tls
1690     PRINT " From internal memory via COM, Pixels";Lxtnt;"x";Lxtnt;"x";Lxtnt;",
                         title,"
1700     IF Chdr$<>"" THEN PRINT Chdr$
1710     IF Dhdr$<>"" THEN PRINT Dhdr$
1720   CASE =1                              ! Get pixels from file
1730     INPUT " Enclose (in """"s) file name to contain pixel pattern?",Fln$
1740     IF Fln$="" THEN STOP
1750     IF POS(Fln$,":")=0 THEN Fln$=Fln$&Msd$
1760     DISP " File named """;Fln$;""" ([";LEN(Fln$);"] characters)";
1770     DISP " is being read from storage"
1780     ASSIGN @Pixsrc TO Fln$;FORMAT OFF
1790     ENTER @Pixsrc;Chdr$,Dhdr$;Lxtnt     ! NB header assigned length of 80
1800     PRINT " Pixels contained in file """;Fln$;""", entitled with"
1810     PRINT Chdr$
1820     PRINT Dhdr$
1830     REDIM Pixl(1:Lxtnt,1:Lxtnt,1:Lxtnt) ! read initial Pixl(*) array
1840     ENTER @Pixsrc;Pixl(*)                ! retreive pixels from file
1850     ASSIGN @Pixsrc TO *                  ! close file
1860     LET Lside=Lxtnt*Qdrnt*Tls            ! actual Pixel side anticipated
1870     PRINT
1880   CASE ELSE                              ! Generate pixels
1890     DISP "How big a capacitor pixel grid in elements/side? ";
1900     INPUT "(even #, max ~20 int addr lmt)",Lside
1910     IF Lside<0 THEN STOP
1920     IF Lside<>SHIFT(SHIFT(Lside,1),-1) THEN
1930       PRINT " Odd";Lside;"Pixel length changed to even";
1940       LET Lside=SHIFT(SHIFT(Lside,1),-1)
1950       PRINT Lside
1960     END IF
1970     IF Lside=0 THEN Lside=2
1980     LET Lxtnt=Lside                      ! initial Pixel side length
1990     LET Lside=Lside*Qdrnt*Tls            ! Pixel side length anticipated
2000     IF Lside>32 THEN PRINT " ... near integer addressing limit"
2010   END SELECT                             ! end Ptrn test
2020   PRINT
2030   IF Tls=2 OR Qdrnt=2 THEN PRINT " Pixels now
                         measures";Lside;"x";Lside;"x";Lside
2040   PRINT " Pattern=";Ptrn;")";Lside;"x";Lside;"x";Lside
2050   IF Tls=1 THEN PRINT "pixels,";
2060   IF Tls=2 THEN PRINT "tiled pixels,";
2070   IF Kond=1 THEN PRINT " insulated or ""D"" field parallel to edge."
2080   IF Kond=2 THEN PRINT " periodic or voltage wrapping around at edges."
2090   !ALLOCATE REAL Dsplc(Lside,Lside,Lside),Potnt(Lside,Lside,Lside)
2100   !***> Initializing
```

```
2110   MAT Diel=(CMPLX(0,0))
2120   DISP "Dielectric sources? ";
2130   DISP "1) (from program) 2) user ";
2140   INPUT "3) by steps 4) lossy/real binary ",Nd
2150   IF Nd=0 THEN Nd=2
2160   SELECT Nd
2170   CASE =1
2180     FOR Ndl=1 TO 9
2190       READ Diel(Ndl)
2200     NEXT Ndl
2210   CASE =2
2220     FOR Ndl=1 TO 9
2230       DISP "Give dielectric complex value at";Ndl;
2240       INPUT "? (or enter (-real,0) if to cease)",Diel(Ndl)
2250       IF REAL(Diel(Ndl))<0 THEN
2260         LET Diel(Ndl)=CMPLX(0,0)
2270         LET Ndl=9
2280       ELSE
2290         PRINT "diel[";Ndl;"]=(";VAL$(DROUND(REAL(Diel(Ndl)),4));",";
2300         PRINT VAL$(DROUND(IMAG(Diel(Ndl)),4));"),";
2310       END IF
2320     NEXT Ndl
2330   CASE =3
2340     INPUT "Complex dielectric value of pixel type ""[1]""?",Ctmp
2350     DISP "Multiplier of progression for each succeeding value ";
2360     INPUT "to fill [2],[3],...,[9] ?",Tmpl
2370     FOR Ndl=1 TO 9
2380       Diel(Ndl)=Ctmp
2390       Ctmp=Ctmp*Tmpl
2400       PRINT "diel[";Ndl;"]=(";VAL$(DROUND(REAL(Diel(Ndl)),4));",";
2410       PRINT VAL$(DROUND(IMAG(Diel(Ndl)),4));"),";
2420     NEXT Ndl
2430   CASE =4
2440     DISP "Constituent [1] is solely imaginary(lossy), ie=(0,_),";
2450     INPUT " what is the value? ",Tmpl
2460     LET Diel(1)=CMPLX(0,Tmpl)
2470     DISP "Constituent [2] is solely real, ie=(_,0),";
2480     INPUT " what is the value? ",Tmpl
2490     LET Diel(2)=CMPLX(Tmpl,0)
2500   CASE ELSE
2510     STOP
2520   END SELECT
2530   PRINT
2540   LET Sprss=1
2550   IF Nodesz<32 THEN
2560     INPUT "Surpress screen listing details, 0) No 1) Yes?",Sprss
2570     IF Sprss<0 THEN STOP
2580   END IF
2590   INPUT "Any overall repeats (0=single manual run)? ",Rep
2600   LET Rep=SHIFT(Rep,-1)                !! double if conjugates
2610   LET Relay(0)=Rep                     ! Manual when Relay=0
2620   LET Relay(1)=SHIFT(Rep,1)+1          ! repeat conjugates
2630   IF Rep<0 THEN STOP
2640   IF Rep=0 THEN LET Rep=1              ! If manual, still go thru once
2650   LET Nsvf=0
```

```
2660   IF Rep>1 THEN
2670     INPUT "Save data in a file? 0=No 1=Yes ",Nsvf
2680     LET Nsvf=BIT(Nsvf,0)
2690     IF Nsvf=0 THEN
2700       LET Fsv$=""
2710     ELSE
2720       INPUT "Name a new file to receive data output ",Fsv$
2730       IF Fsv$<>"" THEN LINPUT "Title or description? (<80) ",Ahdr$
2740     END IF
2750   END IF
2760   INPUT "Desire transpose of pixel grid? 0) No 1) Yes",Pose
2770   IF Pose<0 THEN STOP
2780   LET Pose=1+BIT(Pose,0)
2790   REM " Solution acheived by a sparse matrix reduced pivoting technique"
2800   !***>> Overall repetition, may require additional editing
2810   LET Stmrp=TIMEDATE                    ! Timer for repeat"
2820   LET Kwd=4            ! user has selected to program for 4 data columns
2830   REDIM Graf(1:Rep,1:Kwd)
2840   MAT Graf=(0)                          ! Intialize to zero
2850   FOR Rptr=1 TO Rep
2860     LET Rsw=BIT(Rptr,0)                 !Even=0/Odd=1 switch
2870   !!LET Grpt=Grpt+1                     ! Increment data store counter
2880     LET Grpt=Grpt+Rsw                   !!Increment storage counter(on 2s)
2890     IF Relay(0)<>0 THEN LET Relay(0)=Rptr !Standard option of Relay
2900     MAT Frpx=(0)                        !Reset volume fractions to 0
2910     MAT Diel=CONJG(Diel)                !!conjugation option
2920   !!IF Rptr>0 AND Rptr MOD Lside*Lside=0 THEN MAT Diel=CONJG(Diel)!!Conjg
2930     !**> if Ptrn=0 internal or Ptrn=1 then Pixels  read from file
2940     IF Ptrn=2 THEN CALL Pixl3d_fill
2950     IF Ptrn=3 THEN CALL Pixl3d_rand
2960     IF Ptrn=4 THEN CALL Pixl3d_tilt
2970     IF Ptrn=5 THEN CALL Pixl3d_ellps
2980     IF Ptrn=6 THEN CALL Pixl3d_strat
2990     IF Ptrn=7 THEN CALL Pixl3d_cbox
3000     IF Ptrn=8 THEN CALL Pixl2d_3d
3010     IF Tls=2 THEN
3020       LET Xkin=SIZE(Pixl,1)             ! redimensioning
3030       LET Ykin=SIZE(Pixl,2)
3040       LET Zkin=SIZE(Pixl,3)
3050       LET Nd1=2*(Xkin+Ykin+Zkin) DIV 3 ! ave new dimension
3060       LET Nd2=SHIFT(Xkin*Ykin*Zkin,-3) ! 8*Xkin*Ykin*Zkin
3070       REDIM Pixl(1:1,1:Nd2)             ! shifting Pixl array contents
3080       FOR Xcnt=(Xkin-1) TO 0 STEP -1
3090         FOR Ycnt=Ykin TO 1 STEP -1
3100           LET Pixl(1,1,Xcnt*2*Ykin+Ycnt)=Pixl(1,1,Xcnt*Ykin+Ycnt)
3110         NEXT Ycnt
3120       NEXT Xcnt
3130       REDIM Pixl(1:Nd1,1:Nd1,1:Nd1)     ! set new array dimen
3140       FOR Xcnt=Xkin TO 1 STEP -1        ! tiling 2x2
3150         FOR Ycnt=Ykin TO 1 STEP -1
3160           !LET Itmp=Pixl(1,Xcnt,Ycnt)
3170           LET Xaddr=SHIFT(Xcnt,-1)      ! effective 2* op
3180           LET Yaddr=SHIFT(Ycnt,-1)
3190           LET Pixl(1,Xaddr,Yaddr)=Itmp
3200           LET Pixl(1,Xaddr-1,Yaddr)=Itmp
```

```
3210          LET Pixl(1,Xaddr,Yaddr-1)=Itmp
3220          LET Pixl(1,Xaddr-1,Yaddr-1)=Itmp
3230        NEXT Ycnt
3240      NEXT Xcnt
3250    END IF
3260    IF Qdrnt=2 THEN
3270      LET Nd1=(SIZE(Pixl,1)+SIZE(Pixl,2)+SIZE(Pixl,3)) DIV 3
3280      LET Nd2=SHIFT(Nd2,-1)
3290      REDIM Pixl(1:Nd2,1:Nd2,1:Nd2)        ! redim to dble quad duplic
3300      FOR Xcnt=Nd1 TO 1 STEP -1
3310        LET Xaddr=Nd2+1-Xcnt               ! quad complement X counter
3320        LET Xkin=SHIFT(Xcnt+1,1)           ! effectively DIV 2 op
3330        LET Ykin=BIT(Xcnt+1,0)             ! effectively odd<=>even op
3340        FOR Ycnt=1 TO Nd1
3350          LET Yaddr=Nd2+1-Ycnt             ! quad complement Y counter
3360          LET Itmp=Pixl(1,Xkin,Ycnt+Nd1*Ykin)
3370          LET Pixl(1,Xcnt,Ycnt)=Itmp       ! Itmp takes care of redim elements
3380          LET Pixl(1,Xaddr,Ycnt)=Itmp
3390          LET Pixl(1,Xcnt,Yaddr)=Itmp
3400          LET Pixl(1,Xaddr,Yaddr)=Itmp
3410        NEXT Ycnt
3420      NEXT Xcnt
3430    END IF
3440    LET Lside=SIZE(Pixl,1)                 ! update Pixl extent along edge
3450    LET Px_tot=Lside*Lside*Lside           ! update actual Pixl volume
3460    LET Boxes=SHIFT(Lside,1)               ! 1/2 of edge length in Pixls
3470    IF Boxes<1 THEN PRINT "WARNING! may be too small of a pixel grid"
3480    LET Nodesz=SHIFT(Lside*Lside*(Lside+1),2)-SHIFT(5*Lside,1)+4
3490    !***> Tranpose of Pixel grid
3500    LET Trans=Pose ! if loop then use next line
3510    !FOR Trans=1 TO Pose
3520    IF Trans=2 THEN                        ! Tranpose in @ Xplanes
3530      PRINT " TRANSPOSING about the X direction"
3540      FOR Xcnt=1 TO Lside
3550        FOR Ycnt=1 TO Lside
3560          FOR Zcnt=(Ycnt+1) TO Lside
3570            LET Itmp=Pixl(Xcnt,Zcnt,Ycnt) !swap Ycoordinate<->Zcoordinate
3580            LET Pixl(Xcnt,Zcnt,Ycnt)=Pixl(Xcnt,Ycnt,Zcnt)
3590            LET Pixl(Xcnt,Ycnt,Zcnt)=Itmp
3600          NEXT Zcnt
3610        NEXT Ycnt
3620      NEXT Xcnt
3630    END IF
3640    !***> Evaluation of pixel type volume fractions
3650    IF NOT (Sprss) OR Lside<10 THEN PRINT "  Pixels";Lside;"x";Lside;"x";Lside
3660    FOR Xcnt=1 TO Lside                    !by X-plane sections
3670      IF NOT (Sprss) OR Lside<10 THEN PRINT RPT$(" ",Boxes);"X=";VAL$(Xcnt)
3680      FOR Zcnt=Lside TO 1 STEP -1          !Z printout by rows, largest Z 1st row
3690        FOR Ycnt=1 TO Lside               !Y printout across, increasing Y
3700          LET Frpx(Pixl(Xcnt,Ycnt,Zcnt))=Frpx(Pixl(Xcnt,Ycnt,Zcnt))+1
3710          IF NOT (Sprss) OR Lside<10 THEN PRINT " ";VAL$(Pixl(Xcnt,Ycnt,Zcnt));
3720        NEXT Ycnt
3730        IF NOT (Sprss) OR Lside<10 THEN PRINT
3740      NEXT Zcnt
3750    NEXT Xcnt
```

```
3760      MAT Frpx=Frpx/(Px_tot)
3770      PRINT " Volume %s: ";
3780      FOR Nd=1 TO 9
3790        IF Frpx(Nd)<>0 THEN PRINT PROUND(100*Frpx(Nd),-1);"%=>[";Nd;"],";
3800      NEXT Nd
3810      PRINT
3820      IF Frpx(0)<>0 THEN PRINT "WARNING! check pixels"
3830      DISP " .. wait";Rptr;"of";Rep;".. solving node interact matrix,";
3840      DISP Nodesz;"by";Nodesz;"from time ";TIME$(TIMEDATE)
3850      LET Tmp=TIMEDATE                    ! Benchmarker
3860      !***>  HOP technique of sparse matrix reduction
3870      PRINT " Solving node INTERACTION matrix";Nodesz;"x";Nodesz;"via hopper"
3880      LET Hedge=SHIFT(Lside*Lside,1)+Lside-2 !hopper edge, max interact diff
3890      LET Hmem=(1.0+Hedge)*Hedge/2        ! total hopper memory requirement
3900      LET Hsteps=Nodesz
3910      LET Hpremax=Hmem-Hedge
3920      REDIM Hpiv(1:Hedge),Hpr(1:Hmem)
3930      MAT Hpiv=(CMPLX(0,0))
3940      MAT Hpr=(CMPLX(0,0))
3950      LET Hkm=0                           ! 0,1,3,6.. previous hopper row end
3960      FOR Hnde=1 TO Hedge                 ! Filling hopper work array
3970        IF NOT (Sprss) THEN PRINT " node's";Hnde;" lower neighbors are";
3980        FOR Sctr=0 TO 7                   ! Diagonal or self interact terms
3990          IF Kond=1 THEN CALL Cv3ndi(Hnde,Lside,Sctr,Xt(Sctr),Yt(Sctr),Zt(Sctr))
4000          IF Kond=2 THEN CALL Cv3ndp(Hnde,Lside,Sctr,Xt(Sctr),Yt(Sctr),Zt(Sctr))
4010          LET Kube=(Xt(Sctr)<1 OR Xt(Sctr)>Lside OR Yt(Sctr)<1) !in cube?
4020          LET Kube= NOT (Kube OR Yt(Sctr)>Lside OR Zt(Sctr)<1 OR Zt(Sctr)>Lside)
4030          IF Kube THEN
4040            LET Admt(Sctr)=Diel(Pixl(Xt(Sctr),Yt(Sctr),Zt(Sctr)))
4050            IF Kond=1 THEN                ! adj for insl BC on Pixel grid
4060              LET Hcnr=(Xt(Sctr)=1 OR Xt(Sctr)=Lside)!Pix on corner
4070              LET Hcnr=(Hcnr AND (Yt(Sctr)=1 OR Yt(Sctr)=Lside))
4080              LET Hcnr=(Hcnr AND Zt(Sctr)>1 AND Zt(Sctr)<Lside)
4090              IF Hcnr THEN                ! test if corner
4100                LET Jxt=SHIFT(SHIFT(Zt(Sctr),1),-1)+BIT(BINCMP(Zt(Sctr)),0)
4110                LET Adms1=Diel(Pixl(Xt(Sctr),Yt(Sctr),Zt(Sctr)))
4120                LET Adms2=Diel(Pixl(Xt(Sctr),Yt(Sctr),Jxt))
4130                LET Adms1=Adms1*Adms2/(Adms1+Adms2)
4140                LET Admt(Sctr)=Adms1      ! admittance of path
4150              END IF                      ! end of Hnde=Hcnr test
4160            END IF                        ! end if for Kond=1  test
4170            LET Hpr(Hkm+Hnde)=Hpr(Hkm+Hnde)+. '(Sctr) !self interact
4180            IF BIT(Sctr,0)=0 THEN         ! find out lower Z neighbors
4190              IF NOT (Sprss) THEN
4200                PRINT " (";VAL$(Xt(Sctr));",";VAL$(Yt(Sctr));",";
4210                PRINT VAL$(Zt(Sctr));")@";
4220              END IF
4230              SELECT Kond
4240              CASE =1
4250                LET Hnbr(Sctr)=FNNni(Xt(Sctr),Yt(Sctr),Zt(Sctr),Lside,1)
4260              CASE =2
4270                LET Hnbr(Sctr)=FNNnp(Xt(Sctr),Yt(Sctr),Zt(Sctr),Lside,1)
4280              CASE ELSE
4290                PRINT " out of bounds, boundary condition, detected in HOPper"
4300              END SELECT
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4310              IF NOT (Sprss) THEN PRINT VAL$(Hnbr(Sctr));
4320              IF Hnbr(Sctr)>Hnde THEN PRINT " ???";
4330              IF Hnbr(Sctr)<=Hnde-Hedge THEN PRINT "Node";Hnbr(Sctr);"outside of
                      hopper at";Hnde
4340              IF Hnbr(Sctr)<Hnde AND Hnbr(Sctr)>0 THEN
4350                LET Hpr(Hkm+Hnbr(Sctr))=Hpr(Hkm+Hnbr(Sctr))-Admt(Sctr)!neighbr
4360              END IF
4370            END IF                          ! end if for even Sctr
4380          END IF                            ! end if for Kube
4390       NEXT Sctr
4400       IF NOT (Sprss) THEN PRINT            ! end of output line
4410       LET Hkm=Hkm+Hnde                     ! loop count accumulator
4420    NEXT Hnde                               ! end of set up of work matrix
4430    LET Kcnt=0
4440    IF NOT (Sprss) THEN
4450       FOR Xcnt=1 TO Hedge                  ! printout HOPper
4460          FOR Ycnt=1 TO Xcnt
4470             PRINT "(";VAL$(DROUND(REAL(Hpr(Kcnt+Ycnt)),3));",";
4480             PRINT VAL$(DROUND(IMAG(Hpr(Kcnt+Ycnt)),3));") ";
4490          NEXT Ycnt
4500          PRINT
4510          LET Kcnt=Kcnt+Xcnt
4520       NEXT Xcnt
4530    END IF
4540    FOR Hopped=1 TO Hsteps-1                 ! Let the PIVOTING begin, & drip dry
4550       LET Hnde=Hedge+Hopped                 ! count of oncoming node number
4560       LET Hpiv(1)=CMPLX(1,0)                ! normalize to 1st elment pivot vectr
4570       LET Kcnt=2                            ! convert array storage for 1st colmn
4580       IF Hpr(1)=CMPLX(0,0) THEN             ! don't waste steps if 0
4590          PRINT "1st=0?";
4600          MAT Hpiv=(CMPLX(0,0))
4610       ELSE
4620          LET Hnrm=1/Hpr(1)                  ! set normalizing multiplier
4630          FOR Hcnt=2 TO Hedge                ! set pivot vector
4640             LET Hpiv(Hcnt)=Hpr(Kcnt)*Hnrm
4650             LET Kcnt=Kcnt+Hcnt              ! 2,4,7,11,..@1st elmnt in hoppr row
4660          NEXT Hcnt
4670       END IF
4680       !***> one can output pivot here for backsub later
4690       IF NOT (Sprss) THEN
4700          IF Hnde<=Hsteps+1 THEN
4710             PRINT "feed node";Hnde-1;
4720             FOR Ycnt=1 TO Hedge          ! printout of hopper feed row
4730                PRINT "(";VAL$(DROUND(REAL(Hpr(Hpremax+Ycnt)),3));",";
4740                PRINT VAL$(DROUND(IMAG(Hpr(Hpremax+Ycnt)),3));") ";
4750             NEXT Ycnt
4760             PRINT
4770          END IF                            ! end if for Hnde<Hsteps
4780          PRINT " At reduction";Hopped;"the complex pivots are:"
4790          LET Xcnt=MIN(Hedge,Hsteps-Hopped+1) !significant
4800          FOR Hcnt=Xcnt TO 1 STEP -1
4810             PRINT "{";VAL$(DROUND(REAL(Hpiv(Hcnt)),4));",";
4820             PRINT VAL$(DROUND(IMAG(Hpiv(Hcnt)),4));"}";
4830          NEXT Hcnt
4840          IF Hpiv(1)=CMPLX(0,0) THEN PRINT "?!";
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4850        PRINT
4860        END IF
4870        LET Kcnt=1                    ! initialize filling counter
4880        FOR Xcnt=2 TO Hedge           ! heart of pivoting
4890          IF Hpiv(Xcnt)<>CMPLX(0,0) THEN ! sparseness efficiency =0, no-op
4900            FOR Ycnt=2 TO Xcnt        ! adj each array row with pivot vectr
4910              IF Hpiv(Ycnt)<>CMPLX(0,0) THEN ! sparseness efficiency =0, no-op
4920                LET Hpr(Kcnt+Ycnt)=Hpr(Kcnt+Ycnt)-Hpr(Kcnt+1)*Hpiv(Ycnt)
4930              END IF
4940            NEXT Ycnt
4950          END IF
4960          LET Kcnt=Kcnt+Xcnt          !1,3,6,10,.. gives previous row end
4970        NEXT Xcnt
4980        LET Kcnt=0                    ! initialize filling counter lower
4990        FOR Xcnt=1 TO Hedge-1         ! X,Y refer to hopping counters
5000          FOR Ycnt=1 TO Xcnt          ! hopping along for shake up
5010            LET Hpr(Kcnt+Ycnt)=Hpr(Kcnt+Ycnt+1+Xcnt)
5020          NEXT Ycnt
5030          LET Kcnt=Kcnt+Xcnt
5040        NEXT Xcnt
5050        FOR Ycnt=1 TO Hedge           ! feed hopper, clear last row
5060          LET Hpr(Hpremax+Ycnt)=CMPLX(0,0)
5070        NEXT Ycnt
5080        IF NOT (Sprss) AND Hnde<Hsteps THEN PRINT " node's";Hnde;" lower neighbors
                        are";
5090        FOR Sctr=0 TO 7               ! find neighbors
5100          SELECT Hnde
5110          CASE <Hsteps                ! feed unless over lg array extent
5120            IF Kond=1 THEN CALL Cv3ndi(Hnde,Lside,Sctr,Xt(Sctr),Yt(Sctr),Zt(Sctr))
5130            IF Kond=2 THEN CALL Cv3ndp(Hnde,Lside,Sctr,Xt(Sctr),Yt(Sctr),Zt(Sctr))
5140            LET Kube=(Xt(Sctr)<1 OR Xt(Sctr)>Lside OR Yt(Sctr)<1) !in cube?
5150            LET Kube=(Kube OR Yt(Sctr)>Lside OR Zt(Sctr)<1 OR Zt(Sctr)>Lside)
5160            LET Kube= NOT (Kube)
5170            IF Kube THEN
5180              LET Admt(Sctr)=Diel(Pixl(Xt(Sctr),Yt(Sctr),Zt(Sctr)))
5190              IF Kond=1 THEN          ! adj for insl BC on Pixel grid
5200                LET Hcnr=(Xt(Sctr)=1 OR Xt(Sctr)=Lside)!Pix on corner
5210                LET Hcnr=(Hcnr AND (Yt(Sctr)=1 OR Yt(Sctr)=Lside))
5220                LET Hcnr=(Hcnr AND Zt(Sctr)>1 AND Zt(Sctr)<Lside)
5230                IF Hcnr THEN          ! test if corner
5240                  LET Jxt=SHIFT(SHIFT(Zt(Sctr),1),-1)+BIT(BINCMP(Zt(Sctr)),0)
5250                  LET Adms1=Diel(Pixl(Xt(Sctr),Yt(Sctr),Zt(Sctr)))
5260                  LET Adms2=Diel(Pixl(Xt(Sctr),Yt(Sctr),Jxt))
5270                  LET Adms1=Adms1*Adms2/(Adms1+Adms2)
5280                  LET Admt(Sctr)=Adms1! admittance of path
5290                END IF                ! end of Hnde=Hcnr test
5300              END IF                  ! end if for Kond=1  test
5310              LET Hpr(Hmem)=Hpr(Hmem)+Admt(Sctr)
5320              IF BIT(Sctr,0)=0 THEN   ! find lower Z neighor interactions
5330                IF NOT (Sprss) THEN PRINT "
                        (";VAL$(Xt(Sctr));",";VAL$(Yt(Sctr));",";VAL$(Zt(Sctr));")@";
5340                SELECT Kond
5350                CASE =1
5360                  LET Hnbr(Sctr)=FNNni(Xt(Sctr),Yt(Sctr),Zt(Sctr),Lside,1)
5370                CASE =2
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5380              LET Hnbr(Sctr)=FNNnp(Xt(Sctr),Yt(Sctr),Zt(Sctr),Lside,1)
5390              END SELECT              ! to SELECT Kond
5400              IF NOT (Sprss) THEN PRINT VAL$(Hnbr(Sctr));
5410              IF Hnbr(Sctr)>=Hnde THEN PRINT " ???";
5420              IF Hnbr(Sctr)<=Hnde-Hedge THEN PRINT "Node";Hnbr(Sctr);"outside of
                    hopper at";Hnde
5430              IF Hnbr(Sctr)<Hnde AND Hnbr(Sctr)>0 THEN
5440                LET Hnbr(Sctr)=Hnbr(Sctr)+Hmem-Hnde
5450                LET Hpr(Hnbr(Sctr))=Hpr(Hnbr(Sctr))-Admt(Sctr)
5460              END IF
5470            END IF                    ! end if for even Sctr
5480          END IF                      ! end if in Kube
5490        CASE =Hsteps                  ! special case, exciter electrode
5500          IF BIT(Sctr,0)=0 THEN       ! do on even Sctr
5510            !IF NOT (Sprss) THEN PRINT " ";VAL$(Hsteps);
5520            FOR Xcnt=1 TO Boxes        ! pixels which abut exciter electrode
5530              LET Xkin=SHIFT(Xcnt,-1)+BIT(Sctr,2)-1! X address in Sctr
5540              FOR Ycnt=1 TO Boxes  ! & neighbors
5550                LET Ykin=SHIFT(Ycnt,-1)+BIT(Sctr,1)-1! Y addrss in Sctr
5560                LET Hpr(Hmem)=Hpr(Hmem)+Diel(Pixl(Xkin,Ykin,Lside))
5570                LET Hnbr(Sctr)=Hsteps-1-(Boxes-Ycnt+1)*Boxes+Xcnt
5580                !IF NOT (Sprss) THEN PRINT "@";VAL$(Hnbr(Sctr));!neighbr
5590                LET Hnbr(Sctr)=Hnbr(Sctr)+Hmem-Hnde !rel. to hopper address
5600                Hpr(Hnbr(Sctr))=Hpr(Hnbr(Sctr))-Diel(Pixl(Xkin,Ykin,Lside))
5610              NEXT Ycnt
5620            NEXT Xcnt
5630          END IF                       ! end if even SCTR
5640        END SELECT                     ! to SELECT Hnde
5650      NEXT Sctr
5660      IF NOT (Sprss) AND Hnde<=Hsteps THEN PRINT ! end of print out line
5670    NEXT Hopped
5680    IF NOT (Sprss) THEN
5690      PRINT " Complex hopper funnels down to {";DROUND(REAL(Hpr(1)),4);
5700      PRINT ",";DROUND(IMAG(Hpr(1)),4);"}"
5710    END IF
5720    !***> Hpr(1) contains the end of the interaction reduction
5730    !    LET Hpiv(Hsteps)=1/Hpr(1)      ! backsubstitute for solution vector
5740    !    FOR Hcnt=(Hsteps-1) TO 1 STEP -1
5750    !      LET Hpiv(Hcnt)=0
5760    !      FOR Kcnt=Hcnt TO Hsteps
5770    !        LET Hpiv(Hcnt)=Hpiv(Hcnt)-Pivotstorg(Hcnt,1+Kcnt-Hcnt)*Hpiv(Kcnt)
5780    !      NEXT Kcnt
5790    !    NEXT Hcnt
5800    PRINT "                ... at ";TIME$(TIMEDATE);" inversion excution ";
5810    PRINT "time took";PROUND(TIMEDATE-Tmp,-1);"seconds"
5820    DISP
5830    LET Resp=Hpr(1)/Lside              ! principal diel resp
5840    !***> Pixl displacement field/current & potentials
5850    !  FOR Ycnt=1 TO Lside
5860    !    FOR Xcnt=1 TO Lside
5870    !      Slant=(Xcnt+Ycnt) MOD 2
5880    !      Xaddr=Xcnt-Boxes-Slant         ! (x,y) of node upper to pixel
5890    !      Yaddr=Ycnt-Boxes
5900    !      CALL Xy_to_node(Ndl,Xaddr,Yaddr,Lside,Kond)
5910    !      Xaddr=Xcnt-Boxes+Slant-1       ! (x,y) of node lower to pixel
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5920  !         Yaddr=Ycnt-Boxes-1
5930  !         CALL Xy_to_node(Nd2,Xaddr,Yaddr,Lside,Kond)
5940  !         IF Nd1<>Nd2 AND Nd1>0 AND Nd2>0 THEN
5950  !           Dsplc(Xcnt,Ycnt)=Diel(Pixl(1,Xcnt,Ycnt))*(Hpiv(Nd1)-Hpiv(Nd2))
5960  !           Potnt(Xcnt,Ycnt)=(Hpiv(Nd1)+Hpiv(Nd2))/2
5970  !         END IF
5980  !         IF Nd2=0 AND Nd1>0 THEN
5990  !           Dsplc(Xcnt,Ycnt)=Diel(Pixl(1,Xcnt,Ycnt))*Hpiv(Nd1)
6000  !           Potnt(Xcnt,Ycnt)=Hpiv(Nd1)/2
6010  !         END IF
6020  !       NEXT Xcnt
6030  !     NEXT Ycnt
6040  !***> additional modification of Potential & Displacement array fields
6050  !   IF Kond=1 THEN
6060  !     FOR Ycnt=2 TO (Lside-2) STEP 2
6070  !       FOR Nd=-1 TO 1 STEP 2
6080  !         LET Xcnt=(Nd+1)*Boxes+(Nd=-1)   ! (Xcnt,Ycnt) refer to pixel
6090  !         LET Xaddr=Nd*(Boxes-1)          ! (Xaddr,Yaddr) refer to node
6100  !         LET Yaddr=Ycnt-Boxes
6110  !         CALL Xy_to_node(Nd1,Xaddr,Yaddr+1,Lside,Kond)! node # upper
6120  !         CALL Xy_to_node(Nd2,Xaddr,Yaddr-1,Lside,Kond)! node # lower
6130  !         IF Nd1<>Nd2 AND Nd1>0 AND Nd2>0 THEN ! Evaluate along side nodes
6140  !           LET Tmp1=Diel(Pixl(1,Xcnt,Ycnt+1))! Upper dielectric pixel
6150  !           LET Tmp2=Diel(Pixl(1,Xcnt,Ycnt))! Lower dielectric pixel
6160  !           LET Vt1=Hpiv(Nd1)
6170  !           LET Vt2=Hpiv(Nd2)
6180  !           IF Tmp1<>0 AND Tmp2<>0 THEN Tmp=(Vt1*Tmp1+Vt2*Tmp2)/(Tmp1+Tmp2)
6190  !           LET Potnt(Xcnt,Ycnt+1)=(Vt1+Tmp)/2! Pixl volts
6200  !           LET Potnt(Xcnt,Ycnt)=(Vt2+Tmp)/2
6210  !           IF Tmp1<>0 AND Tmp2<>0 THEN
6220  !              LET Dsplc(Xcnt,Ycnt+1)=(Vt1-Vt2)/(1/Tmp1+1/Tmp2)
6230  !           END IF
6240  !           LET Dsplc(Xcnt,Ycnt)=Dsplc(Xcnt,Ycnt+1)! Displacement mag.
6250  !         END IF
6260  !       NEXT Nd
6270  !     NEXT Ycnt
6280  !   END IF
6290  !   MAT Potnt= Potnt*(Resp)        ! Normalizing to 1 volt across sample
6300  !   MAT Dsplc= Dsplc*(Resp)        ! & sum of displacements along row=diel
6310  !   LET Nd1=1                      ! sign provider for following loop
6320  !   FOR Xcnt=1 TO Lside
6330  !     LET Resp2=Resp2+Nd1*(Dsplc(Xcnt,Boxes)-Dsplc(Xcnt,Boxes+1))
6340  !     LET Nd1=-Nd1
6350  !   NEXT Xcnt
6360  !   LET Resp2=Resp2/2              ! dielectric response perp to E
6370  !***> Should be end of calculations, printouts follow
6380  !***> Printout of the dielectric pixel array
6390     IF NOT (Sprss) AND Lside<10 THEN
6400       PRINT "DIELECTRIC PIXEL ARRAY, 3-dimensional,";Lside;"x";Lside;"x";Lside
6410       FOR Xcnt=1 TO Lside
6420         PRINT RPT$(" ",Lside);"X plane=";VAL$(Xcnt)
6430         FOR Zcnt=Lside TO 1 STEP -1
6440           FOR Ycnt=1 TO Lside
6450             PRINT "(";VAL$(DROUND(REAL(Diel(Pixl(Xcnt,Ycnt,Zcnt))),3));",";
6460             PRINT VAL$(DROUND(IMAG(Diel(Pixl(Xcnt,Ycnt,Zcnt))),3));") ";
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6470            NEXT Ycnt
6480              PRINT
6490           NEXT Zcnt
6500         NEXT Xcnt
6510      END IF
6520    !***> Printout of the hopper array
6530      !****>  Find the series<->parallel factor
6540      LET Ctmp=FNWnr(Diel(*),Frpx(*),Resp,Tmp,9)
6550      PRINT
6560      PRINT "Composite Dielectric Response Tensor Components:"
6570      PRINT " principal=";Resp
6580      PRINT "  & series<->parallel factor =";
6590      PRINT "(";VAL$(DROUND(REAL(Ctmp),4));",";VAL$(DROUND(IMAG(Ctmp),4));")";
6600      PRINT "(+/- ";VAL$(DROUND(100*Tmp,4));"% iteration error)"
6610      PRINT
6620    !  IF Sprss=0 THEN
6630    !     PRINT "PIXEL VOLTAGES 2-dimensional,";Lside;"by";Lside
6640    !     Tmp=FNMatprnt(Potnt(*),-Lside)
6650    !     PRINT "PIXEL DISPLACEMENT FIELD MAGNITIUDES,";Lside;"by";Lside
6660    !     Tmp=FNMatprnt(Dsplc(*),-Lside)
6670    !  END IF
6680        !***> NOTE: Tranpose used then it is an additional cycle to Rptr
6690      !Graf(Grpt,1)=Rptr+Tmp/100
6700      !Graf(Grpt,2)=Frpx(1)
6710      !Graf(Grpt,3)=REAL(Ctmp)          ! save real part of exp ave factor
6720      !Graf(Grpt,4)=IMAG(Ctmp)          ! save imag part of exp ave factor
6730      Graf(Grpt,1)=(Rptr+Tmp/100)*.25+Graf(Grpt,1)+.125
6740      Graf(Grpt,2)=Frpx(1)*.5+Graf(Grpt,2)
6750      Graf(Grpt,3)=REAL(Ctmp)*.5+Graf(Grpt,3)
6760      Graf(Grpt,4)=IMAG(Ctmp)*.5+Graf(Grpt,4)
6770      !NEXT Trans
6780    NEXT Rptr
6790    !***> output repeat calculations
6800    LET Stmrp=TIMEDATE-Stmrp          ! Repeat time elapsed
6810    IF Stmrp>300 THEN BEEP            ! Beep if longer than 5 minutes
6820    IF Rptr>1 THEN PRINT "Finished";Rptr-1;"repeat trials in";Stmrp;"seconds."
6830    LET Bhdr$="("&VAL$(Lside)&"x"&VAL$(Lside)&"x"&VAL$(Lside)&")"
6840    IF Tls=1 THEN LET Bhdr$=Bhdr$&" elmnts"
6850    IF Tls=2 THEN LET Bhdr$=Bhdr$&"/(2x2x2s)"
6860    IF Kond=1 THEN LET Bhdr$=Bhdr$&" InslBC"
6870    IF Kond=2 THEN LET Bhdr$=Bhdr$&" PrdcBC"
6880    LET Bhdr$=Bhdr$&" Sparse"     ! solution by sparse methods
6890    IF Qdrnt=2 THEN LET Bhdr$=Bhdr$&" 4fold"
6900    IF Ptrn=0 THEN Bhdr$=Bhdr$&" intrnl,"
6910    IF Ptrn=1 THEN Bhdr$=Bhdr$&" "&Fln$
6920    IF Ptrn=2 THEN Bhdr$=Bhdr$&" USER,"
6930    IF Ptrn=3 THEN Bhdr$=Bhdr$&" RANDOM,"
6940    IF Ptrn=4 THEN Bhdr$=Bhdr$&" SLANT,"
6950    IF Ptrn=5 THEN Bhdr$=Bhdr$&" ELLIPSE,"
6960    IF Ptrn=6 THEN Bhdr$=Bhdr$&" STRAT,"
6970    IF Ptrn=7 THEN Bhdr$=Bhdr$&" BOXES,"
6980    LET Occp=LEN(Bhdr$)
6990    LET Bhdr$[1+Occp]=RPT$(" ",80-Occp)    ! pad with blanks
7000    LET Bhdr$[60]=" "&DATE$(TIMEDATE)&","&TIME$(TIMEDATE)
7010    LET Dhdr$=Bhdr$
```

```
7020   IF Rep=1 THEN PRINT "  for the case abbreviated .."
7030   IF Rep=1 THEN PRINT Bhdr$
7040   IF Rep>1 THEN
7050     PRINT " Summary of";Grpt;"repeat variations: (as programmed)"
7060     FOR Rptr=1 TO Grpt
7070       PRINT " Case";((Rptr-1) DIV Pose)+1;")",DROUND(Graf(Rptr,1),4),
7080       PRINT DROUND(Graf(Rptr,2),4),DROUND(Graf(Rptr,3),4),
7090       PRINT DROUND(Graf(Rptr,4),4)
7100     NEXT Rptr
7110     IF Nsvf=0 THEN
7120       DISP " Save repeat info (array form,";SIZE(Graf,1);"x";SIZE(Graf,2);
7130       INPUT ")? 0) No 1) Definitely",Nd1
7140     ELSE
7150       LET Nd1=0
7160       IF Fsv$<>"" THEN
7170         REDIM Graf(1:Grpt,1:Kwd)
7180         CREATE Fsv$,1 !<--<DOS if 1 unit
7190         ASSIGN @Savstr TO Fsv$;FORMAT OFF
7200         OUTPUT @Savstr;Ahdr$,Bhdr$,Grpt,Kwd,Graf(*),END
7210         ASSIGN @Savstr TO *
7220       ELSE
7230         Nd1=1
7240       END IF
7250     END IF
7260     IF Nd1=1 THEN
7270       DISP " Enclose (in """"s) new file name to send info vectors to?";
7280       INPUT " (@/null=use old file)",Fln$
7290       IF POS(Fln$,":")=0 THEN Fln$=Fln$&Msd$
7300       LINPUT " Title, (up to 80 characters)",Ahdr$
7310       LET Ahdr$[1+LEN(Ahdr$)]=RPT$(" ",80-LEN(Ahdr$))! pad with blanks
7320       DISP " File named """;Fln$;""" ([";LEN(Fln$);"] characters)";
7330       DISP " to contain repeat info"
7340       PRINT " File """;Fln$;"""'s user and description headers are ";
7350       PRINT "(2 lines):"
7360       PRINT Ahdr$
7370       PRINT Bhdr$
7380       IF Fln$="" OR Nsvf=1 THEN
7390         INPUT "  Enter the filename to be created? null=stop",Fln$
7400         IF Fln$="" THEN STOP
7410         !DISP " Enter file""";Fln$;"""'s storage size limit in bytes (`";
7420         DISP VAL$(256+8*Rep*Pose*Kwd);")";
7430         INPUT "?",Nd1
7440 !!      IF Nd1<1048 THEN Nd1=1048        ! 1 kiloBYTE min (LIF disks)
7450         CREATE Fln$,Nd1
7460       ELSE
7470         IF POS(Fln$,":")=0 THEN Fln$=Fln$&Msd$
7480       END IF
7490       ASSIGN @Infostr TO Fln$;FORMAT OFF
7500       OUTPUT @Infostr;Ahdr$,Bhdr$,Rep,Kwd,Graf(*),END
7510       ASSIGN @Infostr TO *
7520     END IF
7530   END IF
7540   !***> Pixel file output choice
7550   LET Nd1=0
7560 !IF Ptrn<>1 THEN INPUT " Save last pixel grid? 0)No 1)Yes",Nd1
```

```
7570   LET Nd1=0 !!temporary unitl reprogramming done
7580   IF Nd1=1 THEN
7590     DISP " Enclose (in """"s) new file name to send pixel pattern to?";
7600     INPUT " (null=use old file)",Fln$
7610     IF POS(Fln$,":")=0 THEN Fln$=Fln$&Msd$
7620     LINPUT " Title (up to 80 characters) if null then default label",Chdr$
7630     LET Dhdr$=Bhdr$
7640     DISP " File named """;Fln$;""" ([";LEN(Fln$);"] characters)";
7650     DISP " contains the pixel grid"
7660     PRINT " File """;Fln$;"""'s header is "
7670     PRINT Hdr$
7680     IF Fln$<>"" THEN
7690       DISP " Give file""";Fln$;"""'s max capacity limit in bytes";
7700       DISP "? (~";VAL$(128+SHIFT(Px_tot,-1));")";
7710       INPUT " ",Nd1
7720       IF Nd1<256 THEN Nd1=256
7730       CREATE Fln$,Nd1
7740     ELSE
7750       INPUT "  Enter the existing filename?",Fln$
7760       IF POS(Fln$,":")=0 THEN Fln$=Fln$&Msd$
7770     END IF
7780     ASSIGN @Pixstr TO Fln$;FORMAT OFF
7790     OUTPUT @Pixstr;Hdr$,Lside,Pixl(*),END
7800     ASSIGN @Pixstr TO *
7810   END IF
7820   !***> Interaction file output choice
7830   PRINT RPT$(" ",25);"...elapsed";PROUND(TIMEDATE-Start,-1);
7840   PRINT "sec for completion at ";TIME$(TIMEDATE)
7850   PRINT " MEMORY IS";VAL(SYSTEM$("AVAILABLE MEMORY"))/8;"(reals)"
7860   LET Lxtnt=Lside                      ! update COM /Pixel/ ie Pixl(*) size
7870   END
7880   ! ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][
7890   SUB Cv3ndi(INTEGER Nodi,Lszi,Sctri,Xouti,Youti,Zouti)
7900   ! Converts a node number of layering scheme into the (x,y,z)
7910   ! coordinates of neighboring nodes
7920   ! IN    Nodi = node number
7930   ! IN    Lszi = Pixl extent along either X or Y
7940   ! IN    Sctri = selection adjacent Pixl neighbor to node
7950   !         ie, quadrant number from binary (x/0/1 y/0/1 z/0/1)
7960   !         example 5>=>101 or x=1 y=0 z=1 or
7970   !         (0= X lower,Y lower Z lower; 1= X lower,Y lower, Z higher
7980   !          2= X lower, Y higher, Z lower; etc
7990   ! OUT Xouti = X coordinate address outcome
8000   ! OUT Youti = Y coordinate address outcome
8010   ! OUT Zouti = Z coordinate address outcome
8020   ! internal variables:
8030   !  Lyri = a counter for number of layers
8040   !  Swi = an even odd switch
8050   !  Ovri = overfill counter
8060   !  Nodmaxi = maximum node for given Pixel grid size, Lszi
8070   !  Hfszi = half of Pixel grid size, Lszi (then Lszi must be even)
8080   !  Sqvi = 1/4 of square whose edges are: Lszi*Lszi
8090   !  Bilv = the number of nodes between bilayers z={1,2 3,4 5,6 ..
8100     INTEGER Lyri,Swi,Ovri,Nodmaxi,Hfszi,Sqvi,Bilv
8110     LET Sctri=BINAND(Sctri,7)          ! mask only relevant bits
```

```
8120    IF BIT(Lszi,0) THEN PRINT " warning, odd Pixel grid extent"
8130    LET Sqvi=SHIFT(Lszi*Lszi,2)       ! 1/4 of square Lszi*Lszi
8140    LET Bilv=SHIFT(Lszi*Lszi,1)+Lszi-3 !Nodes in bilayer
8150    LET Nodmaxi=Sqvi*(Lszi+1)-SHIFT(5*Lszi,1)+4 !max node #
8160    LET Hfszi=SHIFT(Lszi,1)                ! effectively DIV 2 operation
8170    SELECT Nodi
8180    CASE <1                             ! grounded
8190      LET Xouti=Hfszi
8200      LET Youti=Hfszi
8210      LET Zouti=0
8220    CASE >=Nodmaxi                       ! exciter node
8230      LET Zouti=Lszi+1
8240      LET Youti=Hfszi
8250      LET Xouti=Hfszi
8260    CASE ELSE                           ! node is in cube
8270      LET Lyri=(Nodi-1) DIV Bilv            ! for Bilayer
8280      LET Ovri=(Nodi-1) MOD Bilv            ! for # Nodes in Bilayer itself
8290      LET Swi=(Ovri>=Sqvi)                  ! 0=lower 1=upper in Bilayer
8300      IF Swi THEN LET Ovri=Ovri-Sqvi        ! adjust for # Nodes in upper
8310      LET Zouti=1+SHIFT(Lyri,-1)+Swi+BIT(Sctri,0)
8320      IF Swi=0 THEN                       ! compute according to z level
8330        LET Youti=1+SHIFT(Ovri DIV Hfszi,-1)+BIT(Sctri,1)
8340        LET Xouti=1+SHIFT(Ovri MOD Hfszi,-1)+BIT(Sctri,2)
8350      ELSE
8360        IF Ovri<(Hfszi-1) THEN            ! along Y=1 edge
8370          LET Youti=BIT(Sctri,1)
8380          LET Xouti=SHIFT(Ovri,-1)+2+BIT(Sctri,2)
8390        ELSE                              ! not along Y=1 edge
8400          LET Ovri=Ovri-Hfszi+1
8410          LET Youti=Ovri DIV (Hfszi+1)
8420          LET Xouti=Ovri MOD (Hfszi+1)
8430          IF Youti=Hfszi-1 THEN           ! along Y=Lszi edge
8440            LET Xouti=SHIFT(Xouti,-1)+2+BIT(Sctri,2)
8450          ELSE                            ! somewhere in cube
8460            LET Xouti=SHIFT(Xouti,-1)+BIT(Sctri,2)
8470          END IF
8480          LET Youti=SHIFT(Youti,-1)+2+BIT(Sctri,1)
8490        END IF
8500      END IF
8510    END SELECT
8520    SUBEND
8530    ! ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][
8540    DEF FNNni(INTEGER Xn,Yn,Zn,Lszn,Lup)
8550    ! Returns the node number for Pixel grid network cube
8560    ! of capacitors for case of insulated sides.
8570    ! (Xn,Yn,Zn) 3D coordinates of Pixel leading to the nearest node
8580    ! If Up=1 then Pixl situated above node, else Pixl situated below node
8590    ! Where up is orientation towards exciter electrode
8600    !  & down is orientation towards grounded electrode
8610    INTEGER Ysw,Ndb,Lyr,Lsqhv,Ztyp,Zz
8620    LET Zz=Zn                            ! Copy of Z value for function call
8630    LET Lup=BIT(Lup,0)
8640    LET Lyr=SHIFT(Lszn,1)               ! in essence divides by 2
8650    LET Lsqv=SHIFT(Lszn*Lszn,2)         ! 1/4th of square Lszn*Lszn
8660    IF Xn>0 AND Xn<=Lszn AND Yn>0 AND Yn<=Lszn AND Zz>0 AND Zz<=Lszn THEN
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8670        LET Ndb=1
8680        IF Zz=1 AND Lup THEN LET Ndb=0 !at ground electrode or next exciter
8690        IF Zz=Lszn AND NOT (Lup) THEN LET Ndb=Lsqv*(Lszn+1)-SHIFT(5*Lszn,1)+4
8700        REM above program line contains computation for EXCITER node number
8710        IF Ndb=1 THEN ! Node Numbering. Executes if node not yet assigned
8720          IF Zz<0 THEN Zz=-Zz                ! also entry line if node recalc
8730          LET Ztyp=BIT(Zz+1-Lup,0)         ! 0=no nodes on edge 1=on edge
8740          LET Ndb=(Zz-1-Lup)*Lsqv+SHIFT(Zz-Lup,1)*(Lszn-3)+Ztyp*(2-Lszn)
8750          LET Ndb=Ndb+(Lyr+Ztyp)*SHIFT(Yn+Ztyp-1,1) !node # up to y row
8760          LET Ndb=Ndb+SHIFT(Xn+1-Ztyp,1) ! node # up to x location
8770          IF Ztyp=1 THEN                     ! special cases
8780            IF Yn=1 THEN
8790              LET Ndb=Ndb+1
8800              IF Xn=1 OR Xn=Lszn THEN Zz=-(Zz+(1-SHIFT(Lup,-1)))
8810            END IF
8820            IF Yn=Lszn THEN
8830              LET Ndb=Ndb-1
8840              IF Xn=1 OR Xn=Lszn THEN Zz=-(Zz+(1-SHIFT(Lup,-1)))
8850            END IF
8860          END IF !for(Ztyp=1)
8870        END IF !for(if Ndb=1)
8880        IF Zz<0 THEN GOTO 8720              !recalculate
8890      ELSE
8900        LET Ndb=-1
8910      END IF
8920      RETURN Ndb
8930    FNEND
8940    ! ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][
8950    SUB Pixl3d_rand
8960    !***> Subprogram to create a 3D pixel array of random distribution
8970    ! @$%^%*^&%)! R A N D O M  3 D  P I X E L  G R I D &^#!#%)(%^$*
8980      COM /Pass/Relay(0:7)
8990      COM /Pixel/Chdr$[80],Dhdr$[80],INTEGER Lpix,Pixl(1:20,1:20,1:20)
9000      INTEGER Xp,Yp,Zp,Xq,Yq,Zq,Fill,Frdm,Sqrs,Pxs,Pixtmp,When,Lt,Ldb
9010      INTEGER Knpx,Nrdm,Rot,Dmn
9020    !LET Xq=SIZE(Pixl,1)<>Lpix OR SIZE(Pixl,2)<>Lside OR SIZE(Pixl,3)<>Lpix
9030      REDIM Pixl(1:Lpix,1:Lpix,1:Lpix) !? needed in sub"
9040      PRINT " Enjoy creating a randomized 3D pixel grid whose pixel elements"
9050      PRINT " are labelled 1..9"
9060      LET Nrdm=INT(Relay(0)+.0000001)        !Integer of relay
9070      IF Nrdm=0 THEN                         ! Manual seed
9080        INPUT "Random seed? (integer or neg if to be via timer)",Nrdm
9090        INPUT "Apply to 0) full 3D pixel cube 1) to 2D X-section ",Dmn
9100        IF Dmn>0 THEN
9110          INPUT "Contortions? none=0 compress=.5 elongate=2 ",Vchk
9120          IF Vchk>.25 AND Vchk<.75 THEN Vchk=1
9130          LET Lt=INT(Vchk+.5)
9140        ELSE
9150          LET Lt=0
9160        END IF
9170      ELSE
9180        LET Lt=INT(Relay(2)) MOD 3         ! Test of relay fraction 0,1,2
9190        LET Dmn=INT(.0000001+Relay(4))     ! Relay(4) pony for 2D or 3D
9200        IF Dmn=0 THEN Lt=0
9210      END IF
```

```
9220      LET Ldb=1+(Lt>0)                          ! Doubling factor
9230      IF Nrdm=0 THEN RANDOMIZE INT(TIMEDATE MOD 32767)
9240      IF Nrdm>0 THEN RANDOMIZE Nrdm
9250      LET Fill=0
9260      LET Sqrs=Lpix*Lpix/Ldb
9270      LET Knpx=Sqrs
9280      IF Dmn=0 THEN Knpx=Knpx*Lpix
9290      LET When=0
9300      LET Pxs=0
9310      LET Rq=0
9320      LET Nrdm=SHIFT(INT(Relay(0)+1.000001),1) !!Divide by 2 conj pairing
9330      IF Relay(0)>=1 AND Relay(1)<>0 THEN LET Rq=100*FRACT(Nrdm/Relay(1))
9340      WHILE Fill<Knpx
9350        LET Pxs=Pxs-1                          !Decrement
9360        WHILE Pxs<0
9370          LET When=When+1
9380          IF INT(Relay(0))=0 THEN
9390            DISP "Filling with component [";VAL$(When);"], give volume ";
9400            INPUT "percent (volume fraction * 100) ",Rq
9410          ELSE
9420            IF When>1 THEN Rq=-1               !Fill with rest, after 1st pass
9430          END IF
9440          IF Rq<0 THEN
9450            LET Pxs=Knpx-Fill
9460          ELSE
9470            LET Pxs=INT(Rq*Knpx*.01+.5) MOD Knpx
9480            IF Pxs>Knpx-Fill AND Knpx>Fill THEN Pxs=Knpx-Fill
9490          END IF
9500          PRINT " Component [";VAL$(When);"] is assigned";Pxs*Ldb;"pixels"
9510        END WHILE
9520        IF Pxs>0 AND Dmn>0 THEN
9530          LET Fill=Fill+1                      !Update current square location
9540          LET Zp=((Fill-1) DIV Lpix)+1         !Row of location
9550          LET Yp=Fill-(Zp-1)*Lpix              !Column of location
9560          LET Pixl(1,Zp,Yp)=When               !Assign pixel
9570        END IF
9580        IF Pxs>0 AND Dmn=0 THEN
9590          LET Fill=Fill+1                      !Update current square location
9600          LET Zp=((Fill-1) DIV Sqrs)+1         !Level between electrodes
9610          LET Xq=(Fill-1) MOD Sqrs             !remainder
9620          LET Yp=(Xq DIV Lpix)+1               !Y row in a Z level
9630          LET Xp=(Xq MOD Lpix)+1
9640          LET Pixl(Xp,Yp,Zp)=When              !X location in Y row
9650        END IF
9660      END WHILE
9670  !***> lotto-ing or random mixing
9680      IF Dmn=0 THEN
9690        FOR Fill=1 TO Knpx
9700          LET Frdm=INT(1+RND*Knpx)
9710          IF Fill<>Frdm AND Frdm<=Knpx THEN
9720            LET Zp=((Fill-1) DIV Sqrs)+1
9730            LET Xp=(Fill-1) MOD Sqrs
9740            LET Yp=(Xp DIV Lpix)+1
9750            LET Xp=(Xp MOD Lpix)+1
9760            LET Zq=((Frdm-1) DIV Sqrs)+1
```

```
9770            LET Xq=(Frdm-1) MOD Sqrs
9780            LET Yq=(Xq DIV Lpix)+1
9790            LET Xq=(Xq MOD Lpix)+1
9800            LET Pixtmp=Pixl(Xp,Yp,Zp)
9810            LET Pixl(Xp,Yp,Zp)=Pixl(Xq,Yq,Zq)
9820            LET Pixl(Xq,Yq,Zq)=Pixtmp
9830            !PRINT "r";VAL$(Frdm);"p";VAL$(Pixtmp); !check random sequencing
9840          END IF
9850        NEXT Fill
9860      ELSE
9870        FOR Fill=1 TO Sqrs
9880          LET Frdm=INT(1+RND*Sqrs)
9890          IF Fill<>Frdm AND Frdm<=Sqrs THEN
9900            LET Xp=1
9910            LET Zp=1+((Fill-1) MOD Lpix)
9920            LET Yp=1+((Fill-1) DIV Lpix)
9930            LET Xq=1
9940            LET Zq=1+((Frdm-1) MOD Lpix)
9950            LET Yq=1+((Frdm-1) DIV Lpix)
9960            LET Pixtmp=Pixl(Xp,Yp,Zp)
9970            LET Pixl(Xp,Yp,Zp)=Pixl(Xq,Yq,Zq)
9980            LET Pixl(Xq,Yq,Zq)=Pixtmp
9990            !PRINT "r";VAL$(Frdm);"p";VAL$(Pixtmp); !check random sequencing
10000          END IF
10010        NEXT Fill
10020        FOR Yp=1 TO Lpix                !swap
10030          FOR Zp=(1+Yp) TO Lpix
10040            LET Pixtmp=Pixl(1,Yp,Zp)
10050            LET Pixl(1,Yp,Zp)=Pixl(1,Zp,Yp)
10060            LET Pixl(1,Zp,Yp)=Pixtmp
10070          NEXT Zp
10080        NEXT Yp
10090        IF Ldb>1 THEN
10100          FOR Yp=Lpix TO 1 STEP -1      !Contort expand
10110            LET Yq=SHIFT(Xp+1,1)
10120            FOR Zp=1 TO Lpix
10130              LET Pixl(1,Yp,Zp)=Pixl(1,Yq,Zp)
10140            NEXT Zp
10150          NEXT Yp
10160        END IF
10170        FOR Xp=2 TO Lpix                !Copy over X planes
10180          FOR Yp=1 TO Lpix
10190            FOR Zp=1 TO Lpix
10200              LET Pixl(Xp,Yp,Zp)=Pixl(1,Yp,Zp)
10210            NEXT Zp
10220          NEXT Yp
10230        NEXT Xp
10240        IF Relay(0)=0 THEN INPUT "Rotate about Z axis? 0=N/1=Y ",Rot
10250        IF Rot=1 OR Relay(3)=1 THEN
10260          FOR Zp=1 TO Lpix                !swap
10270            FOR Yp=1 TO Lpix
10280              FOR Xp=(1+Yp) TO Lpix
10290                LET Pixtmp=Pixl(Xp,Yp,Zp)
10300                LET Pixl(Xp,Yp,Zp)=Pixl(Yp,Xp,Zp)
10310                LET Pixl(Yp,Xp,Zp)=Pixtmp
```

```
10320              NEXT Xp
10330            NEXT Yp
10340          NEXT Zp
10350        END IF
10360     END IF                                ! Dmn=0 for 3D or Dmn>1 for 2D
10370 SUBEND
10380 ! ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][ ][
10390 DEF FNWnr(COMPLEX Diel(*),REAL Frpx(*),COMPLEX Din,REAL Alferr,INTEGER Nth)
10400     REM  Object of this function subprogram is to
10410     REM  find the exponential averaging factor (or
10420     REM  percolation related factor) "alf"
10430     REM  from a given set of complex number
10440     REM  dielectric values & fractional volume
10450     REM  weights and effective or resultant
10460     REM  complex dielectric value of composite
10470     REM            written by S. Wallin, 4/91.
10480     REM  The Wiener or exponential averaging factor
10490     REM  is defined as follows:
10500     REM  Diel0(resultant)^Alf = sum {Frpx(k)*Diel(k)^Alf}
10510     REM   where Diel0(resultant) = response of composite
10520     REM           Alf = exponential ave or Wiener or percolation factor
1C530     REM           Frpx(k) = fractional volumes of species k
10540     REM           Diel(k) = (dielectric) response of species k
10550     COM /Pass/Relay(0:7)
10560     INTEGER I,J,K,K1,K2,Kdo,Ns,Lsn,Lst,New
10570     COMPLEX Diel0,Dlog0,Alf,Alf0,C0,C1,C2,C3,Clg,Clg2
10580     LET Ns=Nth
10590     IF Ns<=0 THEN STOP
10600     ALLOCATE COMPLEX Dlog(Ns)
10610     LET Avg=0
10620     LET Diel0=Din
10630     FOR I=1 TO Ns
10640       IF Diel(I)<>CMPLX(0,0) THEN Avg=Avg+Frpx(I)
10650     NEXT I
10660     REM Normalize ACTIVE volume to total 1
10670     FOR I=1 TO Ns
10680       !IF Avg<>0 THEN LET Frpx(I)=Frpx(I)/Avg
10690       IF Diel(I)=CMPLX(0,0) THEN Frpx(I)=0
10700     NEXT I
10710 !PRINT " Species data: (trial#, complex ";CHR$(238);" pair, adj vol wt)"
10720 !FOR I=1 TO Ns
10730  !PRINT " [#";I;"] (";REAL(Diel(I));",";IMAG(Diel(I));")",DROUND(Frpx(I),4)
10740 !NEXT I
10750 !PRINT " [ eff] (";REAL(Diel0);",";IMAG(Diel0);")",1
10760     REM Determination of slope direction by log wt
10770     LET Dlog0=CMPLX(0,0)
10780     IF Diel0<>CMPLX(0,0) THEN Dlog0=LOG(Diel0)
10790     LET Clg=CMPLX(0,0)! Clg=Logarthimic mean
10800     LET Clg2=CMPLX(0,0)
10810     FOR I=1 TO Ns
10820       LET Dlog(I)=CMPLX(0,0)
10830       IF Diel(I)<>CMPLX(0,0) THEN Dlog(I)=LOG(Diel(I))-Dlog0
10840       LET Clg=Clg+Frpx(I)*Dlog(I)
10850       LET Clg2=Clg2+Frpx(I)*Dlog(I)*Dlog(I)
10860     NEXT I
```

```
10870   LET Lsn=-SGN(REAL(Clg))
10880 !PRINT " The logarithmic slope is ";DROUND(REAL(Clg),4);
10890 !PRINT DROUND(IMAG(Clg),4);"indicates ";CHR$(224);" is ";
10900 !IF Lsn=1 THEN !PRINT "positive."
10910 !IF Lsn=0 THEN !PRINT "at zero."
10920 !IF Lsn=-1 THEN !PRINT "negative."
10930   REM Extrema values
10940   LET Lst=0
10950   LET Zst=0
10960   FOR I=1 TO Ns
10970     IF Frpx(I)<>0 THEN
10980       LET Tmp=Lsn*ABS(Diel(I))
10990       IF Tmp>Zst OR Zst=0 THEN
11000         LET Zst=Tmp
11010         LET Lst=I
11020       END IF
11030     END IF
11040   NEXT I
11050   IF Lsn=0 THEN Lst=0
11060   LET Alf=CMPLX(0,0)
11070   IF Lst>0 AND Lst<=Ns+1 THEN
11080     IF Dlog(Lst)<>CMPLX(0,0) THEN Alf=-LOG(Frpx(Lst))/Dlog(Lst)
11090   END IF
11100   LET CO=CMPLX(Lsn,0)
11110   IF Clg2<>CMPLX(0,0) THEN CO=-2*Clg/Clg2!A 2nd guess
11120   LET Wt=ABS(CO)
11130   LET Wt=1/(1+Wt*Wt)!Relative weights for ave the 2 guesses
11140   LET Alf=Alf+Wt*(CO-Alf)!Combined 1st guess
11150 !PRINT "   Guess 1  ";CHR$(224);" = ";
11160 !PRINT DROUND(REAL(Alf),4);DROUND(IMAG(Alf),4)
11170   LET Alf0=CMPLX(0,0)
11180   LET Alferr=1
11190   LET J=2
11200   LET New=0
11210   WHILE Alf<>Alf0 AND J<32 AND Alferr>1.0E 13
11220     IF New=1 THEN
11230       LET Alf0=Alf!Keep track of last iteration
1124C       New=0
11250     END IF
11260     LET C1=CMPLX(0,0)
11270     LET C2=CMPLX(0,0)
11280     LET C3=CMPLX(0,0)
11290     LET K=0!Keep count of non-zero terms
11300     FOR I=1 TO Ns
11310       LET CO=Alf*Dlog(I)
11320       IF ABS(REAL(CO))>700 THEN !Failure possible
11330         LET Alf=-2*Clg/Clg2
11340         LET Alf0=CMPLX(0,0)
11350         LET CO=CMPLX(0,0)
11360         LET C1=CMPLX(0,0)
11370         LET Alferr=0!Set to exit
11380       END IF
11390       IF CO<>CMPLX(0,0) AND Diel(I)<>0 THEN
11400         LET CO=Frpx(I)*EXP(CO)
11410         LET C1=C1+CO
```

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```
11420          LET C2=C2+Dlog(I)*C0
11430          LET C3=C3+Dlog(I)*Dlog(I)*C0
11440          LET K=K+1!Tally another non-zero term
11450        END IF
11460      NEXT I
11470      IF C1<>CMPLX(0,0) AND K>1 THEN ! Log func deriv
11480        REM 0th, 1st, & 2nd logarithmic derivs
11490        LET C2=C2/C1
11500        LET C3=C3/C1-C2*C2
11510        LET C1=LOG(C1)
11520        REM Newton-Raphson estimate via 2nd degree polynomial
11530        LET K1=SGN(REAL(C1))
11540        LET K2=SGN(REAL(C2))
11550        LET C0=CMPLX(0,0)
11560        SELECT K2
11570        CASE 0
11580        !PRINT " o";
11590          IF C3<>CMPLX(0,0) THEN LET C0=-2*C1/C3
11600          IF C0<>CMPLX(0,0) THEN LET Alf=Alf+K1*SQR(C0)
11610        CASE Lsn
11620        !PRINT " +";
11630          LET C0=C2*C2-2*C1*C3
11640          IF C0=CMPLX(0,0) THEN
11650            LET C0=2*C1/C2
11660          ELSE
11670            LET C0=2*C1/(C2+K2*SQR(C0))
11680          END IF
11690          LET Alf=Alf-C0    !New estm of exp factor
11700        CASE -Lsn
11710        !PRINT " -";
11720          LET C0=C2*C2-2*C1*C3
11730          IF C0=CMPLX(0,0) THEN
11740            IF C3<>CMPLX(0,0) THEN LET C0=C2/C3
11750          ELSE
11760            IF C3<>CMPLX(0,0) THEN C0=(C2+K2*SQR(C0))/C3
11770          END IF
11780          LET Alf=Alf-C0    !New estm of exp factor
11790        END SELECT
11800        LET Alferr=ABS(REAL(Alf)-REAL(Alf0))+ABS(IMAG(Alf)-IMAG(Alf0))
11810        IF ABS(REAL(Alf))>700 THEN Alf=CMPLX(Lsn/2,0)-Clg/Clg2/(1+J)!Retry
11820        LET New=1                    !Set for update
11830      END IF
11840      !PRINT " Guess";J;" ";CHR$(224);" = ";Alf;" varied‾";Alferr
11850      LET J=J+1
11860    END WHILE
11870    LET Alferr=ABS(Alf0-Alf)    !Iteration variance
11880    !IF Alferr<>0 THEN !PRINT "  Iteration variance =";Alferr
11890    RETURN Alf
11900 FNEND
   _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _  *  _
```

"DIEL_SITES"
Program in HP BASIC for numeric analysis based on the site model

```
10      REAL Mem0,Tm0
20      LET Tm0=TIMEDATE
30      LET Mem0=INT(.5+VAL(SYSTEM$("AVAILABLE MEMORY")))
40      !   <   <   <   <   <   <     "DIEL_SITES"     >   >   >   >   >   >
50      ! * - * - * - * - * - * - * - * - * - * - * - * - *
60      !   A main program to evaluate a box arrangement of pixel nodes      .
70      !   for the displacement fields and resultant dielectric response    .
80      !   of a composite where nodes and pixels are co-existent.           .
90      !                                                  S. Wallin, June 1991   .
100     ! * - * - * - * - * - * - * - * - * - * - * - *
110     CLEAR SCREEN
120     PRINT "Date: ";DATE$(Tm0);RPT$(" ",48);"Time: ";TIME$(Tm0)
130     PRINT " ";RPT$("  >  ",7);"""DIEL_SIM""";RPT$("  <  ",6);"  <"
140     PRINT RPT$(" ",56);"(S. Wallin, June 1991)"
150     PRINT
160     PRINT "      This program ""DIEL_SIM"" simulates a dielectric composite:";
170     PRINT " a box represented"
180     PRINT "as an interconnected electrical network.  The displacement field";
190     PRINT " (in analogy to "
200     PRINT "current) is a continuous quantity.  The electric field is the";
210     PRINT " voltage drop gra-"
220     PRINT "dient along the displacement field path segments.";
230     PRINT "  Schematically, each pixel is"
240     PRINT "cross joined between faces with a node."
250     PRINT "                                 .  .  .  .  ."
260     PRINT "              Paths            .    |    .";
270     PRINT "         Node at"
280     PRINT "            connect           .____|____.";
290     PRINT "         center"
300     PRINT "            faces             .    |    ."
310     PRINT "                              .    |    ."
320     PRINT "                              .  .  .  .  ."
330     PRINT "The pixels are then interconnected into a nodal network."
340     PRINT "                                      |  <-< Exciter electrode"
350     PRINT "                              ==============="
360     WAIT .1
370     PRINT "                              + + + + + +"
380     WAIT .1
390     PRINT "         X plane             + + + + + +";
400     PRINT "         Y across"
410     WAIT .1
420     PRINT "         on page             + + + + + +";
430     PRINT "         Z to/from"
440     WAIT .1
450     PRINT "         surface             + + + + + +";
460     PRINT "         electrodes"
470     WAIT .1
480     PRINT "                              ==============="
```

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```
490    WAIT .1
500    PRINT "                                              |    <-< Ground electrode"
510    PRINT "Initial memory is";PROUND(Mem0/16,2);
520    PRINT "(available as complex number storage units)."
530    PRINT "[Hint: Use up/down arrow keys to scroll on CRT when paused";
540    PRINT " (halt=Clear"
550    PRINT "I/O & Stop, break=Pause & Stop).]"
560    ! * - * - * - * - * - * - * - * - * - * - * - * - *    !
570    !                                DATA                                    !
580    ! Data is for use as default permittivities                             !
590    DATA 1,0,2,2,4,6,5,8,6,16,7,32,8,64,9,128
600    ! * - * - * - * - * - * - * - * - * - * - * - * - *    !
610    !                           COMmon Memory                               !
620    COM /Info/ INTEGER Dsrc,Kond,Ptrn,Knj,Spcs,Meth,Back,Sgj,Svr,Fln$[80],Msd$[60],COMPL
                       Dlct(0:9)
630    COM /Pass/Relay(0:7)
640    COM /Pixel/ INTEGER Xmax,Ymax,Zmax,Pixl(1:8000),REAL Xscl,Yscl,Zscl
650    COM /Memr/Graf(1:512,1:8),Ahdr$[80],Bhdr$[80],INTEGER Rep,Kwd
660    COM /Titles/Chdr$[80],Dhdr$[80]
670    ! * - * - * - * - * - * - * - * - * - * - * - * - *    !
680    !                              VARIABLES                                 !
690    INTEGER Xadr,Yadr,Zadr,Xcnt,Ycnt,Zcnt
700    INTEGER Axs,Dtl,Face,Infc,Lpiv,Hdig,Hedge,Hlmt,Hmem,Hrel,Hrow,Hclm,Hcnt
710    INTEGER Nd1,Nd2,Ndmax,Nmr,Nwrk,Ovr,Rcyc,Rman,Rptr,Spc0,Zxy
720    REAL Iterr,Mem1,Ntrt,Norm,Tml,Tmv0,Tmv1,Tmcyc,Tmup,Xadm,Yadm,Zadm,Frk(0:9)
730    COMPLEX Admt0,Admt1,Admt2,Alph,Hnrm,Resp
740    DIM Trs$[40],Ws$[250]
750    ! COM /Info/ variable descriptions:
760    !  Dsrc = Dielectric or permittivity selection
770    !  Kond = boundary condition 1) Insulative 2) Periodic or wrap around
780    !  Ptrn = Pixel fill pattern choice
790    !  Knj = permittivity conjugation, 0=none 1=alternating 2=averaged
800    !  Spcs = number of species or types
810    !  Meth = nodal analysis method 1=classic 2=sparseness advantage
820    !  Back = backsubtition indicator 0=off 1=on
830    !  Sgj =  conjugation state +1 or -1
840    !  Svr =  flag to save output on a file
850    !  Fln$ = name of file
860    !  Msd$ = name of mass storage device
870    !  Dlct(*) = array of complex dilectric values
880    ! COM /Pass/ Relay passes information to SUBprograms with 8 reals
890    ! COM /Pixel/ variable descriptions:
900    !  Xmax,Ymax,Zmax = greatest of each pixel address extent
910    !  Pixl(*) = integer array of pixel species for dielectric types
920    !  Xscl,Yscl,Zscl = real scaling factors
930    ! COM /Memr/ variable descriptions:
940    !  Graf(*) = a data output storage array kept after program run
950    !  Ahdr$ = 1st title line for output description
960    !  Bhdr$ = 2nd title line for output description
970    !  Rep = integer of number of repeats or length of array Graf(*)
980    !  Kwd = integer of width of array Graf(*)
990    ! Variables in the MAIN program:
1000   !  Xadr,Yadr,Zadr = integer pixel addresses in (X,Y,Z) coordinates
1010   !  Xcnt,Ycnt,Zcnt = pixel counter addresses in (X,Y,Z) coordinates
1020   !  Axs = 1,2,3 <=> X,Y,Z directions
```

```
1030  !   Dtl = 0 to surpress 1 to print, nodal analysis details
1040  !   Face = integer for 3D axis selection or sector
1050  !   Infc= interfaces tally
1060  !   Lpiv = pivoting occurances
1070  !   Hdig = a counter used for hopper/sparse nodal analysis
1080  !   Hedge = # along edge of hopper/sparse nodal analysis technique
1090  !   Hmem = hopper storage requirement
1100  !   Hrel,Hrow,Hclm,Hcnt = row & column addresses in hopper/sparse tech
1110  !   Nd1 = integer of primary node address
1120  !   Nd2 = integer of a node adjoining primary node
1130  !   Ndmax = node maximum = 1+Xmax*Ymax*Zmax
1140  !   Nwrk = work integer
1150  !   Ovr = integer indicating for overwrite/append output file
1160  !   Rcyc = integer flag to reuse COM /Info/ variables as input
1170  !   Rman = manual flag 0=OFF 1=ON
1180  !   Rptr = integer overall repeat counter
1190  !   Spc0 = integer used in determining species limit
1200  !   Zxy = integer number of pixels on a Z plane, Xmax*Ymax
1210  !   Ntrt = real number of integer value for sparseness memory array
1220  !   Norm = real normalization constant, Zmax/Xmax/Ymax
1230  !   Frk(*) = real array of volume fractions of different types
1240  !   Admt0,Admt1,Admt2 =  complex admittance paths
1250  !   Alph = series<=>parallel, Wiener, or exponential averaging factor
1260  !   Hnrm = normalizing element for hopper pivoting
1270  !   Resp = resultant permittivity
1280  !   Trs$,Ws$ = work string of 40 chars,250
1290  ! Variable arrays to be ALLOCATED
1300  !   Act1(*),Act2(*) = complex nodal interaction array
1310  !   Tca1(*),Tca2(*) = complex inverse of nodal interactoin array
1320  !   Ptn(*) = complex potentials (w/ backsubstition)
1330  !   Endex(*) = complex exciter interactions (w/ backsubstition)
1340  !   Iterr = real iteration error
1350  !   Mem1,Mem0 = real available internal memory for program
1360  !   Tm0,Tm1,Tmv0,Tmv1,Tmcyc,Tmup = real start and stop times
1370  !   Xadm,Yadm,Zadm = pixel face admittance factors
1380  IF Zmax>0 THEN                    ! presumably now a rerun
1390    LET Rcyc=0
1400    IF Kond>0 THEN
1410       INPUT "Rerun at previous settings? 0=no 1=yes (default=0) ",Rcyc
1420    END IF
1430    IF Rcyc<0 THEN STOP             !panic stop
1440    LET Rcyc=(Rcyc>0)
1450  END IF
1460  IF Rcyc THEN                      ! reuse previous inputs, Rcyc=1
1470    LET Zxy=Xmax*Ymax               ! Pixs on a Z level
1480    LET Ndmax=Zxy*Zmax+1            ! Exciter node
1490    LET Xadm=Yscl*Zscl/Xscl         ! X face admittance factor
1500    LET Yadm=Xscl*Zscl/Yscl         ! Y face admittance factor
1510    LET Zadm=Xscl*Yscl/Zscl         ! Z face admittance factor
1520    LET Norm=Zmax/Zadm/Zxy          ! Normalization for permittivity
1530    PRINT "From COM /Memr/ pixel array is";Xmax;"x";Ymax;"x ";VAL$(Zmax);"."
1540    IF Xmax<=0 OR Ymax<=0 OR Zmax<=0 THEN LET Rcyc=0
1550    LET Ws$=""
1560    FOR Xcnt=1 TO Spcs              ! set up a current title
1570       LET Ws$=Ws$&"["&VAL$(Xcnt)&"]s"&"="
```

```
1580        LET Ws$=Ws$&"("&VAL$(DROUND(REAL(Dlct(Xcnt)),3))
1590        LET Ws$=Ws$&","&VAL$(DROUND(IMAG(Dlct(Xcnt)),3))&")"
1600      NEXT Xcnt
1610      LET Ycnt=MIN(LEN(Ws$),75)
1620      LET Ahdr$="Diels "&Ws$[1;Ycnt]
1630    LLSE                               ! get new input info, Rcyc=0
1640      LET Nwrk=0
1650      DISP "IO to be 0) default 1) lab 2) hardisk 3,4) office 5) user defined";
1660      INPUT " (default=0) ",Nwrk
1670      SELECT Nwrk
1680      CASE <0
1690        STOP
1700      CASE =0
1710        LET Msd$=""
1720      CASE =1
1730        LET Msd$=":CS80,700,1"
1740      CASE =2
1750        LET Msd$=":CS80,700,0"
1760      CASE =3
1770        LET Msd$=":CS80,700,0"
1780      CASE =4
1790        LET Msd$=":CS80,703,1"
1800      CASE =5
1810        LINPUT "Name your storage device_ ",Msd$
1820      CASE ELSE
1830        DISP "Mass storage selection too big for menu, defaults"
1840        LET Msd$=""
1850      END SELECT
1860      IF Msd$<>"" THEN PRINT RPT$(" ",48);"mass storage device ";Msd$
1870      PRINT "Indicate Pixel fill pattern:"
1880      PRINT "  0) internal, via COM /Memr/"
1890      PRINT "  1) from file storage"
1900      PRINT "  2) hand fill, (tedious)"
1910      PRINT "  3) random, basic shuffle of pixel iso-sized grains"
1920      PRINT "  4) random, shuffle with dual blocking"
1930      PRINT "  5) ellipsoid, (semi-model of effective medium theory)"
1940      PRINT "  6) correlation, (exponential, power laws)"
1950      PRINT "  7) fractal with evolution by successive generations"
1960      PRINT "     default is currently ";VAL$(Ptrn);"."
1970      LET Nd1=Ptrn                      ! keep track of previous
1980      IF Kond=0 THEN Ptrn=3
1990      DISP "Pixel fill selection? (default=";VAL$(Ptrn);
2000      INPUT ") ",Ptrn
2010      IF Ptrn<0 THEN STOP
2020      IF Ptrn<>Nd1 THEN MAT Relay=(0)   ! zero upon Ptrn change
2030      SELECT Ptrn
2040      CASE =0
2050        IF Xmax<=0 OR Ymax<=0 OR Zmax<=0 THEN
2060          DISP "May have memory error, pixel box measures ";
2070          DISP VAL$(Xmax);"x";VAL$(Ymax);"x";VAL$(Zmax)
2080          STOP
2090        END IF
2100        PRINT "The pixels are from internal memory and measure ";
2110        PRINT VAL$(Xmax);"x";VAL$(Ymax);"x";VAL$(Zmax)
2120      CASE =1
```

```
2130      LINPUT "File source name for Pixels? ",Fln$
2140      IF Fln$="" THEN STOP
2150      IF POS(Fln$,":")=0 THEN Fln$=Fln$&Msd$
2160      DISP "File """;Fln$;""" is being read from storage"
2170      ASSIGN @Pxsrc TO Fln$;FORMAT OFF
2180      ENTER @Pxsrc;Ahdr$;Bhdr$;Xmax;Ymax;Zmax;Xscl;Yscl;Zscl
2190      IF Xmax<=0 OR Ymax<=0 OR Zmax<=0 THEN
2200        DISP """";Fln$;""" may have error, pixel box measures ";
2210        DISP VAL$(Xmax);"x";VAL$(Ymax),"x";VAL$(Zmax)
2220        ASSIGN @Pxsrc TO *
2230        STOP
2240      END IF
2250      IF Xmax<=0 OR Ymax<=0 OR Zmax<=0 THEN PRINT Xmax;"x";Ymax;"x";Zmax;"?"
2260      FOR Xcnt=1 TO Xmax*Ymax*Zmax
2270        ENTER @Pxsrc;Pixl(Xcnt)
2280      NEXT Xcnt
2290      ASSIGN @Pxsrc TO *
2300    END SELECT
2310    IF Ptrn>2 THEN                          !get Pixel limits from user
2320      IF Xmax<1 THEN Xmax=1
2330      DISP "Give X pixel limit, (how many X planes, default=";VAL$(Xmax);
2340      INPUT ")? ",Xmax
2350      IF Xmax<0 THEN STOP
2360      IF Xmax=0 THEN Xmax=1
2370      IF Ymax<1 THEN Ymax=1
2380      DISP "Give Y pixel limit, (how many Y columns/plane,";
2390      DISP " default=";VAL$(Ymax);
2400      INPUT ")? ",Ymax
2410      IF Ymax<0 THEN STOP
2420      IF Ymax=0 THEN Ymax=1
2430      IF Zmax<1 THEN Zmax=1
2440      DISP "Give Z pixel limit, (how many Z rows between electrodes,";
2450      DISP " default ";VAL$(Zm  ;
2460      INPUT ")? ",Zmax
2470      IF Zmax<0 THEN STOP
2480      IF Zmax=0 THEN Zmax=1
2490      IF Xscl<=0 THEN Xscl=1
2500      DISP "Give X pixel scale factor (>0 to inf, default=";VAL$(Xscl);
2510      INPUT ")? ",Xscl
2520      IF Xscl<0 THEN STOP
2530      IF Xscl=0 THEN Xscl=1
2540      IF Yscl<=0 THEN Yscl=1
2550      DISP "Give Y pixel scale factor (>0 to inf, default=";VAL$(Yscl);
2560      INPUT ")? ",Yscl
2570      IF Yscl<0 THEN STOP
2580      IF Yscl=0 THEN Yscl=1
2590      IF Zscl<=0 THEN Zscl=1
2600      DISP "Give Z pixel scale factor (>0 to inf, default=";VAL$(Zscl);
2610      INPUT ")? ",Zscl
2620      IF Zscl<0 THEN STOP
2630      IF Zscl=0 THEN Zscl=1
2640    END IF                          !end if for Ptrn>2 test
2650    PRINT " The scale factors are: X's=";VAL$(DROUND(Xscl,4));
2660    PRINT ", Y's=";VAL$(DROUND(Yscl,4));", & Z's=";VAL$(DROUND(Zscl,4))
2670    IF Kond=0 THEN Kond=1
```

```
2680    DISP "Boundary conditions? 1) Insulated 2) Periodic or";
2690    DISP " wrap around (default=";VAL$(Kond);
2700    INPUT ") ",Kond
2710    IF Kond<0 THEN STOP
2720    LET Kond=(Kond>1)+1
2730    LET Spc0=9                          ! overall species limit set at 9
2740    IF Spcs=0 THEN Spcs=2               ! binary species default
2750    DISP "How many species overall? (<=";VAL$(Spc0);",default=";VAL$(Spcs);
2760    INPUT ")",Spcs                      ! later.. incl option for subspecies
2770    IF Spcs<0 THEN STOP                 ! panic stop
2780    IF Spcs=0 THEN Spcs=2               ! default to binary composite
2790    IF Spcs>Spc0 THEN Spcs=9            ! reset to programming limit
2800    IF Dlct(1)=CMPLX(0,0) THEN LET Dsrc=1 !default
2810    DISP "Permittivi`ies from? 0=intrnl mem 1=prog 2=user ";
2820    IF Spcs=2 THEN DISP "3=binary insl/cond ";
2830    DISP "(default=";VAL$(Dsrc);
2840    INPUT ")",Dsrc
2850    IF Dsrc<0 THEN STOP
2860    IF Dsrc>3 THEN Dsrc=2
2870    IF Dsrc>0 THEN LET Sgj=1            ! reset conjugation state to fresh=+1
2880    SELECT Dsrc
2890    CASE =1
2900      FOR Xcnt=1 TO Spcs
2910        READ Dlct(Xcnt)
2920      NEXT Xcnt
2930    CASE =2
2940      FOR Xcnt=1 TO Spcs
2950        DISP "Complex permittivity for species [";VAL$(Xcnt);
2960        DISP "]s (previous=(";VAL$(DROUND(REAL(Dlct(Xcnt)),4));",";
2970        DISP VAL$(DROUND(IMAG(Dlct(Xcnt)),4));"))";
2980        IF `      ",Dlct(Xcnt)
2990      NEXT Xcnt
3000    CASE =3
3010      FOR Xcnt=1 TO Spcs
3020        IF BIT(Xcnt,0)=0 THEN
3030          LET Iterr=REAL(Dlct(Xcnt))
3040          DISP "For the species [";VAL$(Xcnt);"], give the real part?";
3050          DISP " (previous=";VAL$(DROUND(Iterr,4));
3060          INPUT ") ",Iterr
3070          LET Dlct(Xcnt)=CMPLX(Iterr,0)
3080        ELSE
3090          LET Iterr=IMAG(Dlct(Xcnt))
3100          DISP "For the species [";VAL$(Xcnt); "], give the imaginary";
3110          DISP " (loss) part? (previous=";VAL$(DROUND(Iterr,4));
3120          INPUT ") ",Iterr
3130          LET Dlct(Xcnt)=CMPLX(0,Iterr)
3140        END IF
3150      NEXT Xcnt
3160    END SELECT
3170    IF Meth=0 THEN Meth=2
3180    DISP "Select nodal analysis method 1) classic matrix";
3190    DISP " 2) sparse advantage (default=";VAL$(Meth);
3200    INPUT ") ",Meth
3210    IF Meth<0 THEN STOP                 !panic stop
3220    LET Meth=1+(Meth>1)
```

```
3230      DISP "Backsubstitution, ie backchecking & field mapping? ";
3240      DISP "0=no 1=yes (default=";VAL$(Back);
3250      INPUT ")",Back
3260      IF Back<0 THEN STOP
3270      LET Back=(Back>0)
3280      DISP "How many repeats? (default=";VAL$(Rep);
3290      DISP ", 0=manual, ";VAL$(SIZE(Graf,1));"=max prog)";
3300      INPUT " ",Rep
3310      IF Rep<0 THEN STOP
3320      LET Ws$=""
3330      FOR Xcnt=1 TO Spcs                ! set up title
3340        LET Ws$=Ws$&"["&VAL$(Xcnt)&"]s"&"="
3350        LET Ws$=Ws$&"("&VAL$(DROUND(REAL(Dlct(Xcnt)),3))
3360        LET Ws$=Ws$&","&VAL$(DROUND(IMAG(Dlct(Xcnt)),3))&")"
3370      NEXT Xcnt
3380      LET Ycnt=MIN(LEN(Ws$),75)
3390      LET Ahdr$="Diels "&Ws$[1;Ycnt]
3400      IF Rep>1 THEN
3410        DISP "Conjugate pairing (by 2s)? 0=no 1=alternating 2=averaged ";
3420        DISP "(default=";VAL$(Knj);")";
3430        INPUT " ",Knj
3440        IF Knj<0 THEN STOP
3450        IF Knj>2 THEN Knj=0
3460        DISP "Save repeat information in a file?";
3470        DISP " 0=no 1=yes (default=";VAL$(Svr);
3480        INPUT ") ",Svr
3490        IF Svr<0 THEN STOP               ! panic stop
3500        LET Svr=(Svr>0)
3510        IF Svr THEN
3520          LET Wj$=Fln$                   !for a suggested file naming
3530          IF Ptrn>0 THEN
3540            IF Ptrn=1 THEN Fln$="S"
3550            IF Ptrn=2 THEN Fln$="H"
3560            IF Ptrn=3 THEN Fln$="G"
3570            IF Ptrn=4 THEN Fln$="B"
3580            IF Ptrn=5 THEN Fln$="E"
3590            IF Ptrn=6 THEN Fln$="K"
3600            IF Ptrn=7 THEN Fln$="F"
3610            LET Xcnt=MIN(Xmax,Ymax,Zmax)
3620            LET Ycnt=MAX(Xmax,Ymax,Zmax)
3630            IF Xcnt=Ycnt AND Xmax>9 THEN
3640              Fln$=Fln$&"3D"&VAL$(Xmax)
3650            ELSE
3660              LET Fln$=Fln$&VAL$(Xmax)&VAL$(Ymax)&VAL$(Zmax)
3670            END IF
3680            IF Kond=1 THEN Fln$=Fln$&"S"
3690            IF Kond=2 THEN Fln$=Fln$&"P"
3700          END IF                         ! end if, new suggested filename
3710          IF Ptrn>2 THEN
3720            IF Dlct(2)<>CMPLX(0,0) THEN Admt1=LOG(Dlct(1)/Dlct(2))
3730            LET Admt1=CMPLX(REAL(Admt1)/LOG(10),IMAG(Admt1)*180/PI)*1000
3740            LET Trs$=VAL$(ABS(REAL(Admt1)))
3750            IF ABS(REAL(Admt1))<1000 THEN Trs$="0"&Trs$
3760            LET Fln$=Fln$&Trs$[1;2]
3770            LET Trs$=VAL$(ABS(IMAG(Admt1)))
```

```
3780              IF ABS(REAL(Admtl))<900 THEN Trs$="0"&Trs$
3790              LET Fln$=Fln$&Trs$[1;1]
3800            END IF
3810            OUTPUT KBD;Fln$;
3820            DISP "Verify or name file to receive output (change & enter";
3830            IF Ws$<>"" THEN DISP " or type old=""";Ws$;"""";
3840            LINPUT ") ",Fln$
3850            OUTPUT KBD;Ahdr$;
3860            DISP "Verify or enter a title? (<80";
3870            IF Ahdr$<>"" THEN DISP ", prev run=";Chdr$;
3880            LINPUT ") ",Ahdr$
3890          END IF                        ! end if for Svr
3900        ELSE
3910          LET Knj=0                     ! if no repeats, then no conjugation
3920        END IF                          ! end if for Rep>0
3930      END IF                            ! end if for Rcyc=0
3940      LET Rman=(Rep=0)                  ! manual switch
3950      IF Svr AND Fln$="" THEN Svr=0     ! if nothing change to NO filing
3960      IF Svr THEN                       ! anticipate save output to file
3970        IF POS(Fln$,":")=0 THEN Fln$=Fln$&Msd$ !add mass storage specifier
3980        ON ERROR GOTO 4090              ! error means branch to new file
3990        ASSIGN @Exist TO Fln$
4000        ASSIGN @Exist TO *
4010        OFF ERROR
4020        LET Ovr=0
4030        DISP """";Fln$;""" exists.  Select: 0=skip filing 1=overwrite";
4040        INPUT " 2=append ",Ovr
4050        IF Ovr<0 THEN STOP
4060        IF Ovr>2 THEN Ovr=0
4070        IF Ovr=0 THEN Svr=0
4080        GOTO 4120                       ! branch to end file check
4090        LET Ovr=3                       ! create output file
4100        OFF ERROR
4110        ASSIGN @Exist TO *
4120        REM end of file existance checking
4130      END IF                            ! end if to Svr=save output to file
4140      PRINT "Selections: Pixel pattern =";Ptrn;"& Boundary condition =";Kond
4150      LET Zxy=Xmax*Ymax                 ! Max nodes residing on a Z level
4160      LET Ndmax=Zxy*Zmax+1              ! Exciter node number
4170      LET Xadm=Yscl*Zscl/Xscl          ! X face admittance factor
4180      LET Yadm=Xscl*Zscl/Yscl          ! Y face admittance factor
4190      LET Zadm=Xscl*Yscl/Zscl          ! Z face admittance factor
4200      LET Norm=Zmax/Zadm/Zxy           ! Normalization value
4210      PRINT "The box measures";Xmax;"x";Ymax;"x";Zmax;"pixels giving";
4220      PRINT Ndmax-1;"total."
4230      PRINT "There is a node for each pixel plus the exciter electrode, so";
4240      PRINT " in all ";VAL$(Ndmax);"."
4250      LET Dtl=0                         !Default to no detail
4260      IF Ndmax<37 AND Rman THEN
4270        DISP "View/check nodal ";VAL$(Ndmax);"x";VAL$(Ndmax);" analysis";
4280        INPUT " details? 0=no 1=yes (default=0) ",Dtl
4290        IF Dtl<0 THEN STOP
4300        LET Dtl=(Dtl>0)
4310      END IF                            ! end  if Rep=1 & Ndmax condition
4320      IF Dtl THEN
```

```
4330      PRINT "Nodal analysis numbering scheme"
4340      FOR Xcnt=1 TO Xmax
4350        PRINT RPT$(" ",SHIFT(Ymax,-1));"X=";VAL$(Xcnt)
4360        FOR Zcnt=Zmax TO 1 STEP -1
4370          FOR Ycnt=1 TO Ymax
4380            LET Nwrk=FNODe_mk(Xcnt,Ycnt,Zcnt,Xmax,Ymax,Zmax)
4390            PRINT USING "4D,#";Nwrk
4400            CALL Node_addrs(Nwrk,Xadr,Yadr,Zadr,Xmax,Ymax,Zmax)
4410            IF Xadr<>Xcnt OR Yadr<>Ycnt OR Zadr<>Zcnt THEN
4420              PRINT "(";
4430              IF Xcnt<>Xadr THEN PRINT "X";VAL$(Xcnt);"˜";VAL$(Xadr);
4440              IF Ycnt<>Yadr THEN PRINT "Y";VAL$(Ycnt);"˜";VAL$(Yadr);
4450              IF Zcnt<>Zadr THEN PRINT "Z";VAL$(Zcnt);"˜";VAL$(Zadr);
4460              PRINT ")";
4470            END IF
4480          NEXT Ycnt
4490          PRINT
4500        NEXT Zcnt
4510      NEXT Xcnt
4520    END IF
4530    IF Meth=1 THEN                        !Initialize nodal analysis arrays
4540      ALLOCATE COMPLEX Act1(1:Ndmax,1:Ndmax),Tcal(1:Ndmax,1:Ndmax)
4550      ALLOCATE COMPLEX Ptn(1:Ndmax),Endex(1:Zxy+1),Fluz(1:Ndmax-1)
4560      LET Ntrt=2.0*Ndmax*Ndmax+Ndmax   !number of storage elements
4570    ELSE
4580      LET Hedge=Zxy+1                    !edge units along side of nodal
4590      LET Hmem=(1.0+Hedge)*Hedge*.5     !analysis hopper overall #=Hmem
4600      ALLOCATE COMPLEX Hpiv(1:Hedge),Act2(1:Hmem)
4610      LET Ntrt=(1.0+Ndmax)*Ndmax*.5     !Max nodal storage requirement
4620      ON ERROR GOTO 4670                 !Branch on error to NO backsub
4630      ALLOCATE COMPLEX Tca2(1:Hedge-1,1:Ndmax-1),Ptn(1:Ndmax)
4640      ALLOCATE COMPLEX Endex(1:Hedge),Fluz(1:Ndmax-1)
4650      GOTO 4710                          !else error occured
4660      IF Back=1 THEN
4670        PRINT "Memory too small to save for backsubtitution,";
4680        PRINT " thus NO BACKCHECKING or NO POTENTIALS."
4690      END IF
4700      LET Back=0                         !no backsubstituting
4710      OFF ERROR
4720    END IF
4730    !  =  =  =  =  N O D A L   A N A L Y S I S  =  =  =  =  =
4740    LET Kwd=SIZE(Graf,2)                  ! row size of Graf storage
4750    MAT Graf=(0)                          ! initialize Graf storage
4760    IF Ptrn=2 THEN MAT Relay=(0)          ! zero Relays for manual fill
4770    LET Tmcyc=TIMEDATE                    ! start cycle timer
4780    FOR Rptr=1 TO SHIFT(Rep,-(Knj>0))+Rman! repeat cycles, use conjugation
4790      IF Meth=1 THEN                      ! initialize nodal arrays to zero
4800        MAT Act1=(CMPLX(0,0))
4810        MAT Tcal=(CMPLX(0,0))
4820      ELSE
4830        MAT Act2=(CMPLX(0,0))
4840        IF Back THEN MAT Tca2=(CMPLX(0,0))
4850      END IF
4860    ! FILL PIXELS
4870      IF Ptrn>2 THEN MAT Pixl=(0)         ! initialize pixel array to zero
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4880    LET Nd2=(Knj>0)                    ! use as a test of Knj in SELECT
4890    SELECT Ptrn
4900    CASE =2
4910      CALL Pixs_by_hand
4920    CASE =3
4930      IF NOT (Rcyc OR Rman) AND Rptr=1 THEN ! if multiple calls set Relay(2)
4940        LET Xadr=1
4950        INPUT "Shuffle along the X direction? 0=no 1=yes (default=1) ",Xadr
4960        IF Xadr<0 THEN STOP
4970        LET Xadr=(Xadr=0)
4980        LET Yadr=1
4990        INPUT "Shuffle along the Y direction? 0=no 1=yes (default=1) ",Yadr
5000        IF Yadr<0 THEN STOP
5010        LET Yadr=(Yadr=0)
5020        LET Zadr=1
5030        INPUT "Shuffle along the Z direction? 0=no 1=yes (default=1) ",Zadr
5040        IF Zadr<0 THEN STOP
5050        LET Zadr=(Zadr=0)
5060        REM Relay(0) = volume fractions
5070        REM Relay(1)=seed
5080        LET Relay(2)=SHIFT(Xadr,-2)+SHIFT(Yadr,-1)+Zadr
5090      END IF
5100      IF Rman THEN
5110        Relay(0)=0
5120        Relay(1)=0
5130      ELSE
5140        LET Relay(0)=FRACT(SHIFT(Rptr+Nd2,Nd2)/(Rep+1))!vol frac
5150        LET Relay(1)=Rptr            ! pass to randomize seed
5160      END IF
5170      CALL Pixs_by_random(Spcs)
5180    CASE =4
5190      REM Relay(0) = volume fractions
5200      REM Relay(1)=seed
5210      IF Rman THEN
5220        Relay(0)=0
5230        Relay(1)=0
5240      ELSE
5250        LET Relay(0)=FRACT(SHIFT(Rptr+Nd2,Nd2)/(Rep+1))!vol frac
5260        LET Relay(1)=Rptr            ! pass to randomize seed
5270      END IF
5280      CALL Pixs_by_2block(Spcs)
5290    CASE =5
5300      REM Relay(0) = volume fractions
5310      REM Relay(1,2,3)=ellipse axis
5320      REM Relay(4)
5330      IF NOT Rcyc AND Rptr=1 AND Rep>1 THEN
5340        DISP "Inclusion role? 0)=smaller species, 1)=species #1,";
5350        INPUT " 2)=species #2 ",Relay(4)
5360        IF Relay(4)<0 THEN STOP
5370        LET Relay(1)=1
5380        INPUT "Ellipsoid X axis length? (default=1) ",Relay(1)
5390        LET Relay(2)=1
5400        INPUT "Ellipsoid Y axis length? (default=1) ",Relay(2)
5410        LET Relay(3)=1
5420        INPUT "Ellipsoid Z axis length? (default=1) ",Relay(3)
```

```
5430      END IF
5440      IF Rman THEN
5450        LET Relay(0)=0
5460      ELSE
5470        LET Relay(0)=FRACT(SHIFT(Rptr+Nd2,Nd2)/(Rep+1))!vol frac
5480      END IF
5490      CALL Pixs_by_ellps
5500    CASE =6
5510      REM Relay(0) = volume fractions
5520      REM Relay(1)=seed
5530      REM Relay(2)=correlation select, 0=flat,1=exp,2=inv,3=inv sqr,4=pwr
5540      REM Relay(3)=correlation length or power law
5550      REM Relay(4)=for 1=exp then correl lenght, for 4=pwr then power
5560      IF NOT Rcyc AND Rptr=1 AND Rep>1 THEN
5570        DISP "Corrrelation? none=0 expon=1 inverse=2 inv square=3";
5580        DISP " power law=4 (default=";VAL$(Relay(2));
5590        INPUT ")",Relay(2)
5600        IF Relay(2)=1 THEN
5610          DISP "Correlation length? (in pixel units, default=";
5620          DISP VAL$(Relay(3));
5630          INPUT ")",Relay(3)
5640        END IF
5650        IF Relay(2)=4 THEN
5660          DISP "Power law? (1=inverse 2=inv square, default=";
5670          DISP VAL$(Relay(3));
5680          INPUT ")",Relay(3)
5690        END IF
5700      END IF
5710      IF Rman THEN
5720        Relay(0)=0
5730        Relay(1)=0
5740      ELSE
5750        LET Relay(0)=FRACT(SHIFT(Rptr+Nd2,Nd2)/(Rep+1))!vol frac
5760        LET Relay(1)=Rptr                ! pass to randomize seed
5770      END IF
5780      CALL Pix_by_correlat
5790    CASE =7
5800      REM Relay(0) = volume fractions
5810      REM Relay(1)=seed
5820      REM Relay(2)=number of generations of evolving
5830      IF NOT Rcyc AND Rptr=1 AND Rep>1 THEN
5840        DISP "Maintain constant parent to descendent";
5850        DISP " ratios? Vary=0 Fixed=1 (default=";VAL$(Relay(2));
5860        INPUT ")",Relay(2)
5870        DISP "Number of generations of evolution?";
5880        DISP " (self determine=0, default=";VAL$(Relay(3));
5890        INPUT ")",Relay(3)
5900        DISP "STARTER/CONVERGENCE species? (default=";VAL$(Relay(4));
5910        INPUT ")",Relay(4)
5920        DISP "What is fractional chance of parents descending";
5930        DISP " to other species? (default=";VAL$(FRACT(Relay(5)));
5940        INPUT ")",Relay(5)
5950      END IF
5960      IF Rman THEN
5970        LET Relay(0)=0
```

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5980          LET Relay(1)=0
5990          LET Relay(2)=0
6000          LET Relay(3)=0
6010          LET Relay(4)=0
6020          LET Relay(5)=0
6030        ELSE
6040          LET Relay(0)=FRACT(SHIFT(Rptr+Nd2,Nd2)/(Rep+1))!vol frac
6050          LET Relay(1)=Rptr              ! pass to randomize seed
6060        END IF
6070        CALL Pixs_by_evolv(Spcs)
6080      END SELECT
6090      LET Infc=0                        !Initialize interface tally
6100      MAT Frk=(0)                        !Initialize volume fractions
6110      FOR Nwrk=1 TO Ndmax-1             !Tally up pixel types
6120        IF Pixl(Nwrk)>0 THEN LET Frk(Pixl(Nwrk))=Frk(Pixl(Nwrk))+1
6130      NEXT Nwrk
6140      MAT Frk=Frk/(Ndmax-1)              !convert to vol fractions
6150      IF Rptr<3 THEN                     !print out pixel array
6160        PRINT "The pixel box array";Xmax;"x";Ymax;"x";Zmax;
6170        PRINT "contains the types:"
6180        FOR Xcnt=1 TO Xmax
6190          PRINT RPT$(" ",Ymax);"X=";VAL$(Xcnt)
6200          FOR Zcnt=Zmax TO 1 STEP -1
6210            FOR Ycnt=1 TO Ymax
6220              LET Nwrk=FNOde_mk(Xcnt,Ycnt,Zcnt,Xmax,Ymax,Zmax)
6230              PRINT USING "DD,#";Pixl(Nwrk)
6240            NEXT Ycnt
6250            PRINT
6260          NEXT Zcnt
6270        NEXT Xcnt
6280      END IF
6290      PRINT " Volume fractions are: "
6300      FOR Xcnt=1 TO Spcs
6310        PRINT "[";VAL$(Xcnt);"]s have ";VAL$(DROUND(Frk(Xcnt),4));
6320        IF Xcnt<Spcs THEN PRINT ",";
6330      NEXT Xcnt
6340      PRINT
6350      PRINT "Species permittivities: ";
6360      FOR Xcnt=1 TO Spcs
6370        PRINT " [";VAL$(Xcnt);"]s=(";VAL$(DROUND(REAL(Dlct(Xcnt)),4));",";
6380        PRINT VAL$(DROUND(IMAG(Dlct(Xcnt)),4));")";
6390      NEXT Xcnt
6400      PRINT
6410      IF Dtl THEN PRINT "Principal node & participating neighbor nodes:"
6420      IF Dtl THEN PRINT " Node [ 0] touches";
6430      LET Hdig=1
6440      FOR Nd2=1 TO Zxy               !Z=1 level nodes touching ground
6450        IF Dtl THEN PRINT USING """ [("",DD,"")]"",#";Nd2
6460        LET Admt0=Dlct(Pixl(Nd2))*Zadm!only path admittance to ground
6470        IF Meth=1 THEN LET Act1(Nd2,Nd2)=Admt0
6480        IF Meth=2 THEN LET Act2(Hdig)=Admt0
6490        LET Hdig=Hdig+Nd2+1            !1,3,6,10,15.. diagonal elements
6500      NEXT Nd2
6510      IF Dtl THEN PRINT
6520      IF Meth=2 THEN
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```
6530        LET Tmv0=TIMEDATE            !clock nodal analysis, Meth=2
6540        DISP " ..wait,";Rptr;"of ";VAL$(SHIFT(Rep,-(Knj>0))+Rman);
6550        DISP ", solve";Ndmax;"nodes >@";TIME$(Tmv0)
6560     END IF
6570     LET Lpiv=0                      !pivoting occurances, initialize
6580     LET Hdig=1                      !1,3,6,10,15.. diagonal elements
6590     FOR Nd1=1 TO Ndmax-1            !Range thru all pixel block nodes
6600       IF Dtl THEN PRINT USING """Node ["",DD,""] touches"",#";Nd1
6610       CALL Node_addrs(Nd1,Xadr,Yadr,Zadr,Xmax,Ymax,Zmax)!(X,Y,Z) of node
6620       LET Admt1=Dlct(Pixl(Nd1))     !Admittance in principal node
6630       FOR Axs=1 TO 3                !(1,2,3)<=>(x,y,z) axes
6640         FOR Face=0 TO 1            ! 0=lower 1=upper face wrt choosen axis
6650           LET Nd2=-1              !Intialize as no known node
6660           IF Face THEN           !IF Face(t)=1 (upper face)
6670             SELECT Axs
6680             CASE =1
6690               IF Xadr<Xmax THEN Nd2=Nd1+1 !ordinary neighbor
6700               IF Xadr=Xmax AND Kond=2 THEN Nd2=Nd1-Xmax+1 !wrap periodic X
6710             CASE =2
6720               IF Yadr<Ymax THEN Nd2=Nd1+Xmax
6730               IF Yadr=Ymax AND Kond=2 THEN Nd2=Nd1-Zxy+Xmax !wrap periodic
6740             CASE =3
6750               IF Zadr<Zmax THEN Nd2=Nd1+Zxy
6760               IF Zadr=Zmax THEN Nd2=Ndmax !exciter electrode is neighbor
6770             END SELECT
6780           ELSE                    !else, Face=0 (lower face)
6790             SELECT Axs
6800             CASE =1
6810               IF Xadr>1 THEN Nd2=Nd1-1
6820               IF Xadr=1 AND Kond=2 THEN Nd2=Nd1+Xmax-1 !wrap periodic X
6830             CASE =2
6840               IF Yadr>1 THEN Nd2=Nd1-Xmax
6850               IF Yadr=1 AND Kond=2 THEN Nd2=Nd1+Zxy-Xmax !wrap periodic Y
6860             CASE =3
6870               IF Zadr>1 THEN Nd2=Nd1-Zxy
6880               IF Zadr=1 THEN Nd2=0    !ground electrode is neighbor
6890             END SELECT
6900           END IF                    !end if, Face(t)
6910           IF Dtl THEN PRINT USING """ ["",DD,""]"",#";Nd2
6920           IF Nd2>0 AND Nd1<>Nd2 AND Nd2<Ndmax THEN !a decent neighbor
6930             LET Admt2=Dlct(Pixl(Nd2))!Admittance
6940             LET Admt0=Admt1+Admt2      ! path admittance
6950             IF Pixl(Nd1)<>Pixl(Nd2) THEN Infc=Infc+1 !tally up interfaces
6960             IF Admt0<>CMPLX(0,0) THEN
6970               LET Admt0=Admt1*Admt2/Admt0
6980               IF Axs=1 THEN Admt0=Admt0*Xadm
6990               IF Axs=2 THEN Admt0=Admt0*Yadm
7000               IF Axs=3 THEN Admt0=Admt0*Zadm
7010               IF Meth=1 THEN
7020                 LET Act1(Nd1,Nd1)=Act1(Nd1,Nd1)+Admt0 !self interact
7030                 LET Act1(Nd1,Nd2)=Act1(Nd1,Nd2)-Admt0 !neighbor interact
7040               ELSE                    !else Meth=2, hopper/sparseness tech
7050                 LET Hrel=Nd2-Nd1 !Nd2's address relv to diag element
7060                 IF Nd1<=Hedge THEN !fill hopper
7070                   LET Act2(Hdig)=Act2(Hdig)+Admt0 !Nd1 self interact
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7080                     IF Hrel<0 THEN     !ie Nd2<Nd1, neighbor interact
7090                        LET Act2(Hdig+Hrel)=Act2(Hdig+Hrel)-Admt0
7100                     END IF
7110                   ELSE                 !else w/ hopper/sparseness analysis
7120                     LET Act2(Hmem)=Act2(Hmem)+Admt0
7130                     IF Hrel<0 AND Hrel+Hedge>0 THEN !good neighbors, go ahead
7140                        LET Act2(Hmem+Hrel)=Act2(Hmem+Hrel)-Admt0
7150                     END IF
7160                   END IF              ! end if Nd1>Hedge
7170                 END IF                !Meth
7180               END IF                  !On Admittances non-zero
7190             END IF                    !end if, Nd2 is decent neihbor
7200             IF Meth=2 AND Nd2=Ndmax THEN !if path to exciter electrode
7210               LET Act2(Hmem)=Act2(Hmem)+Dlct(Pixl(Nd1))*Zadm
7220             END IF
7230           NEXT Face
7240         NEXT Axs
7250         IF Dtl THEN PRINT
7260         IF Dtl AND Meth=2 THEN
7270           PRINT USING """ Feed ["",DD,""]""",#";Nd1
7280           IF Nd1<=Hedge THEN Hlmt=Hdig-Nd1+1
7290           IF Nd1>Hedge THEN Hlmt=Hmem-Hedge+1
7300           FOR Hclm=Hlmt TO Hdig
7310             PRINT USING """("",4A,#";VAL$(REAL(Act2(Hclm)))
7320             PRINT USING ""","",4A,"")""",#";VAL$(IMAG(Act2(Hclm)))
7330             IF Hclm-Hlmt MOD 6=5 THEN PRINT !start a new line
7340           NEXT Hclm
7350           IF Hclm-Hlmt MOD 6<>0 THEN PRINT
7360         END IF                        !end if, Dtl
7370         IF Meth=2 AND Nd1>=Hedge THEN !start hopper reduction
7380           LET Lpiv=Lpiv+1             !# pivoting occurances
7390           MAT Hpiv=(CMPLX(0,0))
7400           LET Hpiv(1)=CMPLX(1,0)
7410           IF Act2(1)<>CMPLX(0,0) THEN !initialize pivoting vector
7420             LET Hnrm=1/Act2(1)         !normalizing factor
7430             LET Hclm=2                 !relative address counter
7440             IF Dtl THEN PRINT " Piv (";VAL$(Lpiv);"} (1,0)";
7450             FOR Hrow=2 TO Hedge        !set pivot vector
7460               LET Hpiv(Hrow)=Act2(Hclm)*Hnrm
7470               IF Back THEN Tca2(Hrow-1,Lpiv)=Hpiv(Hrow)
7480               IF Dtl THEN              !print out pivots
7490                 PRINT USING """("",4A,#";VAL$(REAL(Hpiv(Hrow)))
7500                 PRINT USING ""","",4A,"")""",#";VAL$(IMAG(Hpiv(Hrow)))
7510               END IF
7520               LET Hclm=Hclm+Hrow        !2,4.7,11,16.. row start
7530             NEXT Hrow
7540             IF Dtl THEN PRINT
7550           END IF                      !end if, pivot setting
7560           LET Hcnt=1                  !end of row counter
7570           FOR Hrow=2 TO Hedge         !heart of pivoting
7580             IF Hpiv(Hrow)<>CMPLX(0,0) THEN !go ahead
7590               FOR Hclm=2 TO Hrow       !adj @ row with pivots
7600                 LET Nmr=Hcnt+Hclm
7610                 LET Act2(Nmr)=Act2(Nmr)-Act2(Hcnt+1)*Hpiv(Hclm)
7620               NEXT Hclm
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7630            END IF
7640            LET Hcnt=Hcnt+Hrow         !1,3,6,10.. gives row ends
7650          NEXT Hrow
7660        IF Dtl THEN
7670          LET Hcnt=0
7680          FOR Nmr=1 TO Hedge          !dump Act2 array
7690            PRINT USING """  Hop act<"",DD,"">"",#";Nmr
7700            FOR Hclm=1 TO Nmr
7710              PRINT USING """("",4A,#";VAL$(REAL(Act2(Hclm+Hcnt)))
7720              PRINT USING ""","",4A,"")""",#";VAL$(IMAG(Act2(Hclm+Hcnt)))
7730              IF Hclm MOD 6=0 THEN PRINT  !start a new line
7740            NEXT Hclm
7750            IF Hclm MOD 6<>1 THEN PRINT
7760            LET Hcnt=Hcnt+Nmr          !0,1,3,6,10,15.. diags
7770          NEXT Nmr
7780        END IF                        !end if Dtl, Act array dump
7790        LET Hcnt=0                    !ref address to end of previous row
7800        FOR Hrow=1 TO Hedge-1         !shakedown for hopper
7810          FOR Hclm=1 TO Hrow
7820            LET Nmr=Hcnt+Hclm
7830            LET Act2(Nmr)=Act2(Nmr+1+Hrow)
7840          NEXT Hclm
7850          LET Hcnt=Hcnt+Hrow          !0,1,3,6,10,15.. row ends
7860        NEXT Hrow                     !ready to feed hooper
7870        FOR Hclm=Hmem+1-Hedge TO Hmem
7880          LET Act2(Hclm)=CMPLX(0,0) !zero to feed new elements
7890        NEXT Hclm
7900      END IF                          !end if for Nd1>Hedge
7910      IF Nd1<Hedge THEN Hdig=Hdig+Nd1+1 !1,3,6,10.. row end
7920    NEXT Nd1
7930    LET Nd1=Ndmax                     !Exciter node
7940    IF Dtl THEN PRINT USING """Node ["",DD,""] touches"",#";Nd1
7950    IF Back THEN MAT Endex=(CMPLX(0,0))  !initialize exciter interact
7960    FOR Nd2=Ndmax-Zxy TO Ndmax-1     !Z=Zmax level nodes to exciter
7970      IF Dtl THEN PRINT USING """ ["",DD,""]"",#";Nd2
7980      LET Admt0=Dlct(Pixl(Nd2))*Zadm!path admittance to exciter
7990      LET Hrel=Nd2-Nd1                !relative hopper address
8000      IF Meth=1 THEN
8010        LET Act1(Nd1,Nd1)=Act1(Nd1,Nd1)+Admt0
8020        LET Act1(Nd2,Nd2)=Act1(Nd2,Nd2)+Admt0
8030        LET Act1(Nd1,Nd2)=Act1(Nd1,Nd2)-Admt0
8040        LET Act1(Nd2,Nd1)=Act1(Nd2,Nd1)-Admt0
8050      ELSE
8060        LET Act2(Hmem)=Act2(Hmem)+Admt0
8070        IF Hrel+Hedge>0 THEN          !good neighbor to interact
8080          LET Act2(Hmem+Hrel)=Act2(Hmem+Hrel)-Admt0
8090        END IF
8100      END IF                          !end if Meth
8110      IF Back THEN                    !save exciter interactions
8120        LET Endex(Zxy+1)=Endex(Zxy+1)+Admt0 !self exciter
8130        LET Endex(Zxy+1+Hrel)=Endex(Zxy+1+Hrel)-Admt0 !neighbor to exciter
8140      END IF
8150    NEXT Nd2
8160    IF Dtl THEN PRINT
8170    IF Dtl AND Meth=2 THEN
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```
8180        PRINT USING """ Feed {"",DD,""]""",#";Nd1
8190        LET Hlmt=Hmem-Hedge+1
8200        FOR Hclm=Hlmt TO Hdig
8210          PRINT USING """("",4A,#";VAL$(REAL(Act2(Hclm)))
8220          PRINT USING ""","",4A,"")""",#";VAL$(IMAG(Act2(Hclm)))
8230          IF Hclm-Hlmt MOD 6=5 THEN PRINT   !start a new line
8240        NEXT Hclm
8250        IF Hclm-Hlmt MOD 6<>0 THEN PRINT
8260      END IF                          ! end if Dtl
8270      IF Meth=1 THEN
8280        LET Tmv0=TIMEDATE             !Clock nodal analysis, Meth=1
8290        DISP " ..wait,";Rptr;"of ";VAL$(SHIFT(Rep,-(Knj>0))+Rman);
8300        DISP ", solve";Ndmax;"nodes from ";TIME$(Tmv0)
8310        MAT Tca1=INV(Act1)            !solving nodal analysis matrix
8320      ELSE
8330        FOR Hlmt=Hedge TO 2 STEP -1   !play out hopper to funnel it down
8340          LET Lpiv=Lpiv+1             !# of pivoting occurances
8350          MAT Hpiv=(CMPLX(0,0))
8360          LET Hpiv(1)=CMPLX(1,0)
8370          IF Act2(1)<>CMPLX(0,0) THEN !initialize pivoting vector
8380            LET Hnrm=1/Act2(1)        !normalizing factor
8390            IF Dtl THEN PRINT " Piv {";VAL$(Lpiv);"} (1,0)";
8400            LET Hclm=2                !relative address counter
8410            FOR Hrow=2 TO Hlmt        !set pivot vector
8420              LET Hpiv(Hrow)=Act2(Hclm)*Hnrm
8430              IF Back THEN Tca2(Hrow-1,Lpiv)=Hpiv(Hrow)
8440              IF Dtl THEN             !print out pivots
8450                PRINT USING """("",4A,#";VAL$(REAL(Hpiv(Hrow)))
8460                PRINT USING ""","",4A,"")""",#";VAL$(IMAG(Hpiv(Hrow)))
8470              END IF
8480              LET Hclm=Hclm+Hrow      !2,4,7,11,16.. row starts
8490            NEXT Hrow
8500            IF Dtl THEN PRINT
8510          END IF                      !end if, pivot setting
8520          LET Hcnt=1                  !end of row counter
8530          FOR Hrow=2 TO Hlmt          !heart of pivoting
8540            IF Hpiv(Hrow)<>CMPLX(0,0) THEN !go ahead
8550              FOR Hclm=2 TO Hrow      !adj @ row with pivots
8560                LET Nmr=Hcnt+Hclm
8570                LET Act2(Nmr)=Act2(Nmr)-Act2(Hcnt+1)*Hpiv(Hclm)
8580              NEXT Hclm
8590            END IF
8600            LET Hcnt=Hcnt+Hrow        !1,3,6,10,15.. row ends
8610          NEXT Hrow
8620          IF Dtl THEN
8630            LET Hcnt=0
8640            FOR Nmr=1 TO Hlmt         !dump Act2 array
8650              PRINT USING """  Hop act<"",DD,"">""",#";Nmr
8660              FOR Hclm=1 TO Nmr
8670                PRINT USING """("",4A,#";VAL$(REAL(Act2(Hclm+Hcnt)))
8680                PRINT USING ""","",4A,"")""",#";VAL$(IMAG(Act2(Hclm+Hcnt)))
8690                IF Hclm MOD 6=0 THEN PRINT   !start a new line
8700              NEXT Hclm
8710              IF Hclm MOD 6<>1 THEN PRINT
8720              LET Hcnt=Hcnt+Nmr       !0,1,3,6,10,15.. diags
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8730          NEXT Nmr
8740          END IF                      !end if Dtl, Act array dump
8750          LET Hcnt=0                  !ref address to end of previous row
8760          FOR Hrow=1 TO Hlmt-1        !shakedown for hopper
8770            FOR Hclm=1 TO Hrow
8780              LET Nmr=Hcnt+Hclm
8790              LET Act2(Nmr)=Act2(Nmr+1+Hrow)
8800            NEXT Hclm
8810            LET Hcnt=Hcnt+Hrow         !0,1,3,6,10,15.. row ends
8820          NEXT Hrow
8830          FOR Hclm=Hcnt+1 TO Hcnt+Hlmt
8840            LET Act2(Hclm)=CMPLX(0,0) !zero last Hopper row
8850          NEXT Hclm
8860        NEXT Hlmt
8870      END IF                          !end if Meth choices
8880      LET Tmv1=TIMEDATE
8890      DISP ">";TIME$(Tmv1-Tmv0);"<";
8900      IF Dtl THEN
8910        PRINT "Nodal analysis solution required elapsed time of ";
8920        PRINT TIME$(Tmv1-Tmv0);"."
8930      END IF
8940      IF Dtl AND Meth=1 THEN          !Printout of nodal analysis array
8950        PRINT "Contents of classic nodal analysis array";Ndmax;"x ";
8960        PRINT VAL$(Ndmax);", starting at node [1,1].."
8970        FOR Nd1=1 TO Ndmax
8980          LET Admt2=CMPLX(0,0)        !initialize nodal row accumulation
8990          PRINT USING """["",DD,"",*]"",#";Nd1
9000          FOR Nd2=1 TO Ndmax
9010            LET Admt2=Admt2+Act1(Nd1,Nd2)
9020            PRINT USING """(""",4A,#";VAL$(REAL(Act1(Nd1,Nd2)))
9030            PRINT USING """"","",4A,"")"",#";VAL$(IMAG(Act1(Nd1,Nd2)))
9040            IF Nd2 MOD 6=0 THEN PRINT !start a new line
9050          NEXT Nd2
9060          PRINT USING """@("",5A,#";VAL$(REAL(Admt2))
9070          PRINT USING """"","",5A,"")""";VAL$(IMAG(Admt2))
9080        NEXT Nd1
9090      END IF                          !end if Dtl & Meth=1
9100      IF Dtl AND Meth=2 THEN
9110        PRINT USING """  FinalHopAct<"",DD,"">"",#";Nmr
9120        PRINT USING """("",5A,#";VAL$(REAL(Act2(1)))
9130        PRINT USING """"","",5A,"")""";VAL$(IMAG(Act2(1)))
9140      END IF                          ! end if Dtl
9150      LET Hnrm=CMPLX(1,0)             ! anticipated normed current
9160      IF Meth=1 THEN
9170        MAT Ptn=Tcal(*,Ndmax)        !potentials, exciter at (1,~)
9180        IF Back THEN                  !check on exciter
9190          LET Hnrm=CMPLX(0,0)         !node current
9200          FOR Nd1=0 TO Zxy
9210            LET Hnrm=Hnrm+Ptn(Ndmax-Nd1)*Endex(Zxy+1-Nd1)
9220          NEXT Nd1
9230        END IF
9240        LET Resp=Tcal(Ndmax,Ndmax)    !Resultant permittivity
9250        IF Resp<>CMPLX(0,0) THEN LET Resp=2*Norm/Resp
9260      ELSE                            !else do Meth=2
9270        IF Back THEN
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9280            MAT Ptn=(CMPLX(0,0))
9290            IF Act2(1)<>CMPLX(0,0) THEN LET Ptn(Ndmax)=1/Act2(1)
9300            FOR Nd1=Lpiv TO 1 STEP -1         !backtrack node potentials
9310              LET Hlmt=MIN(Hedge-1,Ndmax-Nd1)
9320              FOR Hclm=1 TO Hlmt
9330                LET Nmr=Nd1+Hclm                 !Tca2 node number
9340                LET Ptn(Nd1)=Ptn(Nd1)-Tca2(Hclm,Nd1)*Ptn(Nmr)
9350              NEXT Hclm
9360            NEXT Nd1
9370            LET Hnrm=CMPLX(0,0)                !node current
9380            FOR Nd1=0 TO Zxy
9390              LET Hnrm=Hnrm+Ptn(Ndmax-Nd1)*Endex(Hedge-Nd1)
9400            NEXT Nd1
9410          END IF                              !end if, back
9420          LET Resp=2*Norm*Act2(1)             !Resultant permittivity
9430        END IF                                !end if Meth
9440      IF Back THEN Resp=Resp*Hnrm             !backsubstition correction
9450      IF Back OR Meth=1 THEN                  !presumably arrays exist
9460        MAT Fluz=(CMPLX(0,0))                 !for displacement flux lines
9470        FOR Nd1=1 TO Ndmax-1
9480          LET Admt1=Dlct(Pixl(Nd1))
9490          LET Nd2=Nd1-Zxy                     !lower node neighbor
9500          IF Nd2<1 THEN
9510            LET Fluz(Nd1)=.5*Admt1*Ptn(Nd1)   !admittance to ground
9520          ELSE
9530            LET Admt2=Dlct(Pixl(Nd2))         !neighbor admittance
9540            LET Admt0=Admt1+Admt2
9550            IF Admt0<>CMPLX(0,0) THEN
9560              LET Admt0=Admt1*Admt2/Admt0
9570              LET Admt0=(Ptn(Nd1)-Ptn(Nd2))*Admt0
9580              LET Fluz(Nd1)=.5*Admt0
9590            END IF
9600          END IF                              !end if, Nd2<1
9610          LET Nd2=Nd1+Zxy                     !upper node neighbor
9620          IF Nd2>=Ndmax THEN                  !admittance to exciter
9630            LET Fluz(Nd1)=Fluz(Nd1)+.5*Admt1*(Ptn(Ndmax)-Ptn(Nd1))
9640          ELSE
9650            LET Admt2=Dlct(Pixl(Nd2))         !neighbor admittance
9660            LET Admt0=Admt1+Admt2
9670            IF Admt0<>CMPLX(0,0) THEN
9680              LET Admt0=Admt1*Admt2/Admt0
9690              LET Admt0=(Ptn(Nd2)-Ptn(Nd1))*Admt0
9700              LET Fluz(Nd1)=Fluz(Nd1)+.5*Admt0
9710            END IF
9720          END IF                              !end if, Nd2>=Ndmax
9730        NEXT Nd1
9740      END IF                                  !end if, Back or Meth=1
9750      IF Rman AND (Meth=1 OR Back) THEN
9760        IF REAL(Ptn(Ndmax))<>0 THEN MAT Ptn=Ptn/(REAL(Ptn(Ndmax)))
9770        PRINT "Potentials: at exciter node ";
9780        PRINT USING """("",5A,#";VAL$(REAL(Ptn(Ndmax)))
9790        PRINT USING ""","",5A,"")""";VAL$(IMAG(Ptn(Ndmax)))
9800        FOR Xcnt=1 TO Xmax
9810          PRINT " Cross section, X=";VAL$(Xcnt)
9820          FOR Zcnt=Zmax TO 1 STEP -1
```

```
9830          FOR Ycnt=1 TO Ymax
9840            LET Nwrk=FNOde_mk(Xcnt,Ycnt,Zcnt,Xmax,Ymax,Zmax)
9850            PRINT USING """("",5A,#";VAL$(REAL(Ptn(Nwrk)))
9860            PRINT USING ""","",5A,"")"",#";VAL$(IMAG(Ptn(Nwrk)))
9870            IF Ycnt MOD 5=0 THEN PRINT
9880          NEXT Ycnt
9890          IF Ycnt MOD 5<>1 THEN PRINT
9900        NEXT Zcnt
9910      NEXT Xcnt
9920      PRINT "Displacement fluxes:  exciter node normalized to (1,0)"
9930      LET Admt2=CMPLX(0,0)
9940      FOR Xcnt=1 TO Xmax
9950        PRINT " Cross section, X=";VAL$(Xcnt)
9960        FOR Zcnt=Zmax TO 1 STEP -1
9970          FOR Ycnt=1 TO Ymax
9980            LET Nwrk=FNOde_mk(Xcnt,Ycnt,Zcnt,Xmax,Ymax,Zmax)
9990          ! PRINT USING """("",5A,#";VAL$(REAL(Fluz(Nwrk)))
10000         ! PRINT USING ""","",5A,"")"",#";VAL$(IMAG(Fluz(Nwrk)))
10010           LET Nmr=INT(.5+4*Zxy*REAL(Fluz(Nwrk)))
10020           LET Nd2=7-SHIFT(Nmr+1,1)
10030           IF Nd2>0 THEN Nmr=Nmr+Nd2   !roughly centered
10040           FOR Nd1=1 TO 13            !print real flux
10050             IF Nd1<Nd2 THEN PRINT " ";
10060             IF Nd1>=Nd2 AND Nd1<Nmr THEN PRINT """";
10070             IF Nd1>Nmr THEN PRINT " ";
10080           NEXT Nd1
10090           IF Ycnt MOD 5=0 THEN PRINT
10100           LET Admt2=Admt2+Fluz(Nwrk)
10110         NEXT Ycnt
10120         IF Ycnt MOD 5<>1 THEN PRINT
10130       NEXT Zcnt
10140     NEXT Xcnt
10150     LET Admt2=Admt2/Zmax
10160     PRINT "Average displacement flux through a plane";
10170     PRINT " perpendicular to the electrodes is "
10180     PRINT "   (";VAL$(DROUND(REAL(Admt2),4));
10190     PRINT ",";VAL$(DROUND(IMAG(Admt2),4));")"
10200   END IF                            ! end if for Rman output
10210   PRINT " Resultant permittivity is (";REAL(Resp);",";IMAG(Resp);") & it's"
10220   LET Alph=FNWnr(Dlct(*),Frk(*),Resp,Iterr,Spcs)
10230   IF IMAG(Alph)<>Relay(7) THEN
10240     IF REAL(Alph)<>Relay(6) THEN
10250       PRINT " fail? to pass both cmplx parts of exp av";
10260     ELSE
10270       PRINT " fail? to pass imag part of the exp ave";
10280     END IF
10290     PRINT " factr via FNWnr, now using Relay(6&7)"
10300     LET Alph=CMPLX(Relay(6),Relay(7))
10310   END IF
10320   PRINT " exponential averaging (also Wiener or series<->parallel)";
10330   PRINT " factor is"
10340   PRINT "   (";REAL(Alph);",";IMAG(Alph);")."
10350   IF Ndmax>1 THEN PRINT " Interfaces/pixel=";VAL$(DROUND(Infc/(Ndmax-1),4));
10360   IF Back THEN PRINT " & backsubst correction=";VAL$(ABS(Hnrm-CMPLX(1,0)))
10370   REM Output each cycle to internal storage array
```

```
10380    IF Knj=2 THEN                    ! averaged cases of conjugation pairs
10390      LET Nwrk=SHIFT(Rptr+1,1)      ! effective 1,1,2,2,3,3..
10400      LET Graf(Nwrk,1)=(Nwrk+Iterr)*.5+Graf(Nwrk,1)
10410      LET Graf(Nwrk,2)=Frk(1)*.5+Graf(Nwrk,2)
10420      LET Graf(Nwrk,3)=REAL(Alph)*.5+Graf(Nwrk,3)
10430      LET Graf(Nwrk,4)=IMAG(Alph)*.5+Graf(Nwrk,4)
10440      LET Graf(Nwrk,5)=REAL(Resp)*.5+Graf(Nwrk,5)
10450      LET Graf(Nwrk,6)=IMAG(Resp)*.5+Graf(Nwrk,6)
10460      IF Ndmax>1 THEN LET Graf(Nwrk,7)=Infc/(Ndmax-1)
10470      IF Ptrn=5 THEN                  !other information programmed
10480        LET Graf(Nwrk,8)=Relay(4)*.5+Graf(Nwrk,8) !ellipse roles
10490      ELSE
10500        LET Graf(Nwrk,8)=Relay(2)*.5+Graf(Nwrk,8)
10510      END IF
10520    ELSE                            ! consequetive cases, no averaging
10530      LET Graf(Rptr,1)=Rptr+Iterr
10540      LET Graf(Rptr,2)=Frk(1)
10550      LET Graf(Rptr,3)=REAL(Alph)
10560      LET Graf(Rptr,4)=IMAG(Alph)
10570      LET Graf(Rptr,5)=REAL(Resp)
10580      LET Graf(Rptr,6)=IMAG(Resp)
10590      IF Ndmax>1 THEN LET Graf(Rptr,7)=Sgj*Infc/(Ndmax-1)
10600      IF Ptrn=5 THEN                  ! other programmed information
10610        LET Graf(Rptr,8)=Relay(4) ! ellipse role
10620      ELSE
10630       !LET Graf(Rptr,8)=Relay(2) ! shuffle choice
10640        LET Graf(Rptr,8)=Tmv1-Tmv0 ! matrix inversion time
10650      END IF
10660    END IF                          ! end if, Knj=2
10670    IF Rep>0 THEN SOUND 1,100,10,.04 ! low audible tone per Rptr cycle
10680    LET Tmup=Tmcyc+(TIMEDATE-Tmcyc)*(SHIFT(Rep,-(Knj>0))+Rman)/Rptr+4
10690    IF Knj>0 THEN                    !conjugate on altn Rptr after data done
10700      MAT Dlct=CONJG(Dlct)
10710      LET Sgj=-Sgj
10720    END IF
10730    DISP " finis ¯";TIME$(Tmup);" ";
10740    DISP USING "AAAAAA,#";DATE$(Tmup)
10750 NEXT Rptr
10760 IF Sgj=-1 THEN                    !hopefully unCONJGates
10770    MAT Dlct=CONJG(Dlct)
10780    LET Sgj=1
10790 END IF
10800 !  =  =  =  =  S U M M A R Y   O U T P U T  =  =  =  =  =
10810 DISP
10820 LET Bhdr$="PIXonNODE "
10830 LET Bhdr$=Bhdr$&"SIZ=["&VAL$(Xmax)&"x"&VAL$(Ymax)&"x"&VAL$(Zmax)&"] "
10840 LET Bhdr$=Bhdr$&"SCL="&VAL$(DROUND(Xscl,3))&","
10850 LET Bhdr$=Bhdr$&VAL$(DROUND(Yscl,3))&","&VAL$(DROUND(Zscl,3))&" "
10860 IF Kond=1 THEN Bhdr$=Bhdr$&"InslBC "
10870 IF Kond=2 THEN Bhdr$=Bhdr$&"PrdcBC "
10880 IF Meth=1 THEN Bhdr$=Bhdr$&"Trad "
10890 IF Meth=2 THEN Bhdr$=Bhdr$&"Spar "
10900 IF Ptrn=0 THEN Bhdr$=Bhdr$&"from prev "
10910 IF Ptrn=1 THEN Bhdr$=Bhdr$&"from """&Fln$&""" "
10920 IF Ptrn=2 THEN Bhdr$=Bhdr$&"from USER "
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10930 IF Ptrn=3 THEN Bhdr$=Bhdr$&"RANDOM "
10940 IF Ptrn=4 THEN Bhdr$=Bhdr$&"FRACTAL "
10950 IF Ptrn=5 THEN Bhdr$=Bhdr$&"ELLIPS "
10960 IF Knj=0 THEN Bhdr$=Bhdr$&"NO * "
10970 IF Knj=1 THEN Bhdr$=Bhdr$&"ALT* "
10980 IF Knj=2 THEN Bhdr$=Bhdr$&"AVG* "
10990 IF LEN(Bhdr$)<80 THEN Bhdr$[1+LEN(Bhdr$)]=RPT$(" ",80-LEN(Bhdr$))
11000 LET Trs$=TIME$(TIMEDATE)
11010 LET Ws$=DATE$(TIMEDATE)&" "&Trs$[1;5]
11020 LET Bhdr$[81-LEN(Ws$)]=Ws$              ! Tack time & date to end
11030 IF Rep>1 THEN
11040   PRINT "Summary of repeat cycles: (may be reprogrammed)"
11050   PRINT " TRY.err, VOL FRACTs, REAL, IMAG ALPHA,";
11060   PRINT " REAL, IMAG PERMITTIVITY, & more"
11070   FOR Rptr=1 TO SHIFT(Rep,-(Knj=1))
11080     PRINT "#";VAL$(Rptr);".)";
11090     FOR Xcnt=1 TO Kwd
11100       PRINT USING "X,10A,#";VAL$(DROUND(Graf(Rptr,Xcnt),4))
11110     NEXT Xcnt
11120     PRINT
11130   NEXT Rptr
11140   IF Svr THEN
11150     LET Nmr=SIZE(Graf,1)*SIZE(Graf,2) !memory elements (@8 bytes)
11160     IF Ovr=3 THEN CREATE Fln$,Nmr*8.0+256.0 !for HFS
11170     !IF Ovr=3 THEN CREATE Fln$,1         !for LIF or DOS
11180     LET Nmr=SHIFT(Rep,-(Knj=1))          !length of array Graf
11190     REDIM Graf(1:Nmr,1:Kwd)              !REDIM necessary to size COM output
11200     ASSIGN @Savgraf TO Fln$;FORMAT OFF
11210     IF Ovr=1 OR Ovr=3 THEN
11220       OUTPUT @Savgraf;Ahdr$,Bhdr$,Nmr,Kwd,Graf(*)
11230       OUTPUT @Savgraf;Dlct(*),Xmax,Ymax,Zmax,Xscl,Yscl,Zscl,END
11240     END IF
11250     IF Ovr=2 THEN                        ! append only
11260       ON END @Savgraf GOTO 11300
11270       REM read until end
11280       ENTER @Savgraf;Nwrk               ! read by integers (ie 2 bytes)
11290       GOTO 11270
11300       REM at file end now append
11310       OFF END @Savgraf
11320       OUTPUT @Savgraf;Ahdr$,Bhdr$,Nmr,Kwd,Graf(*)
11330       OUTPUT @Savgraf;Dlct(*),Xmax,Ymax,Zmax,Xscl,Yscl,Zscl,END
11340     END IF                               ! end if to append
11350     ASSIGN @Savgraf TO *
11360   END IF
11370 END IF
11380 LET Chdr$=Ahdr$                          !save titling
11390 LET Dhdr$=Bhdr$
11400 LET Mem1=INT(.5+VAL(SYSTEM$("AVAILABLE MEMORY")))
11410 PRINT "New memory used is";PROUND((Mem0-Mem1)/16,2);"& memory";
11420 PRINT " remaining is";PROUND(Mem1/16,2);"in complex units."
11430 LET Tm1=TIMEDATE
11440 PRINT "TOTAL ELAPSED TIME: ";TIME$(Tm1-Tm0)
11450 PRINT "Date: ";DATE$(Tm1);RPT$(" _ ",7);"FINIS";
11460 PRINT RPT$(" _ ",7);"Time: ";TIME$(Tm1)
11470 SOUND 1,132,14,.2                        ! last call, tell user done
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11480 WAIT .25
11490 SOUND 1,110,15,.5
11500 DISP "Last nodal analysis solution cycle required elapsed time of ";
11510 DISP TIME$(Tmv1-Tmv0);"."
11520 END
11530 !    [    ]    [    ]    [    FNOde_mk    ]    (    ]    [    ]    [    ]
11540 DEF FNOde_mk(INTEGER Xmk,Ymk,Zmk,Xbig,Ybig,Zbig)
11550 ! This function returns the node number for the box Pixel grid
11560 ! Xmk,Ymk,Zmk = the address coordinates of the pixel
11570 ! Xbig,Ybig,Zbig = the Pixel extent in each direction
11580    INTEGER Ndmk! Node number
11590    IF Zmk>0 AND Zmk<=Zbig THEN Ndmk=Xmk+((Ymk-1)+(Zmk-1)*Ybig)*Xbig
11600    IF Zmk<0 THEN Ndmk=0                  !Ground electrode
11610    IF Zmk>Zbig THEN Ndmk=Xbig*Ybig*Zbig+1 !Exciter electrode
11620    IF Xmk<1 OR Xmk>Xbig OR Ymk<1 OR Ymk>Ybig THEN Ndmk=-1
11630    RETURN Ndmk
11640 FNEND
11650 !    [    ]    [    ]    [    SUB Nodeaddrs    [    ]    [    ]    [    ]
11660 SUB Node_addrs(INTEGER Ndsrc,Xxx,Yyy,Zzz,Xlmt,Ylmt,Zlmt)
11670 ! This subroutine returns the (X,Y,Z) addresses for a node number
11680 ! Ndsrc = the node number IN variable
11690 ! Xxx,Yyy,Zzz = the Pixel addresses in each direction OUT variable
11700 ! Xlmt,Ylmt,Zlmt = the Pixel extent in each direction IN variable
11710 ! Sqrxy = the size of a XY plane
11720 ! Ndnd = maximum node
11730 ! Rrr = remaiders, work integer
11740    INTEGER Rrr,Ndnd,Sqrss
11750    LET Sqrxy=Xlmt*Ylmt
11760    LET Ndnd=Sqrxy*Zlmt+1
11770    IF Ndsrc>0 AND Ndsrc<Ndnd THEN
11780      LET Zzz=1+(Ndsrc-1) DIV Sqrxy
11790      LET Rrr=(Ndsrc-1) MOD Sqrxy
11800      LET Yyy=1+(Rrr DIV Xlmt)
11810      LET Xxx=1+(Rrr MOD Xlmt)
11820    ELSE
11830      LET Xxx=SHIFT(Xlmt,1)
11840      LET Yyy=SHIFT(Ylmt,1)
11850      IF Ndsrc>=Ndnd THEN Zzz=Zlmt+1
11860      IF Ndsrc<1 THEN Zzz=0
11870    END IF
11880 SUBEND
11890 !    [    ]    [    ]    function FNWnr    [    ]    [    ]    [    ]
11900 DEF FNWnr(COMPLEX Diel(*),REAL Frpx(*),COMPLEX Din,REAL Alferr,INTEGER Nth)
11910    REM   Object of this function subprogram is to
11920    REM   find the exponential averaging factor (or
11930    REM   percolation related factor) "alf"
11940    REM   from a given set of complex number
11950    REM   dielectric values & fractional volume
11960    REM   weights and effective or resultant
11970    REM   complex dielectric value of composite
11980    REM            written by S. Wallin, 4/91.
11990    REM   The Wiener or exponential averaging factor
12000    REM   is defined as follows:
12010    REM   Diel0(resultant)^Alf = sum {Frpx(k)*Diel(k)^Alf}
12020    REM    where Diel0(resultant) = response of composite
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12030   REM          Alf = exponential ave or Wiener or percolation factor
12040   REM          Frpx(k) = fractional volumes of species k
12050   REM          Diel(k) = (dielectric) response of species k
12060   COM /Pass/Relay(0:7)
12070   INTEGER I,J,K,K1,K2,Kdo,Ns,Lsn,Lst,New
12080   COMPLEX Diel0,Dlog0,Alf,Alf0,C0,C1,C2,C3,Clg,Clg2
12090   LET Ns=Nth
12100   IF Ns<=0 THEN STOP
12110   ALLOCATE COMPLEX Dlog(Ns)
12120   LET Avg=0
12130   LET Diel0=Din
12140   FOR I=1 TO Ns
12150     IF Diel(I)<>CMPLX(0,0) THEN Avg=Avg+Frpx(I)
12160   NEXT I
12170   REM Normalize ACTIVE volume to total 1
12180   FOR I=1 TO Ns
12190     !IF Avg<>0 THEN LET Frpx(I)=Frpx(I)/Avg
12200     IF Diel(I)=CMPLX(0,0) THEN Frpx(I)=0
12210   NEXT I
12220 !PRINT " Species data: (trial#, complex ";CHR$(238);" pair, adj vol wt)"
12230 !FOR I=1 TO Ns
12240  !PRINT " [#";I;"] (";REAL(Diel(I));",";IMAG(Diel(I));")",DROUND(Frpx(I),4)
12250 !NEXT I
12260 !PRINT " [ eff] (";REAL(Diel0);",";IMAG(Diel0);")",1
12270   REM Determination of slope direction by log wt
12280   LET Dlog0=CMPLX(0,0)
12290   IF Diel0<>CMPLX(0,0) THEN Dlog0=LOG(Diel0)
12300   LET Clg=CMPLX(0,0)! Clg=Logarthimic mean
12310   LET Clg2=CMPLX(0,0)
12320   FOR I=1 TO Ns
12330     LET Dlog(I)=CMPLX(0,0)
12340     IF Diel(I)<>CMPLX(0,0) THEN Dlog(I)=LOG(Diel(I))-Dlog0
12350     LET Clg=Clg+Frpx(I)*Dlog(I)
12360     LET Clg2=Clg2+Frpx(I)*Dlog(I)*Dlog(I)
12370   NEXT I
12380   LET Lsn=-SGN(REAL(Clg))
12390 !PRINT " The logarithmic slope is ";DROUND(REAL(Clg),4);
12400 !PRINT DROUND(IMAG(Clg),4);"indicates ";CHR$(224);" is ";
12410 !IF Lsn=1 THEN !PRINT "positive."
12420 !IF Lsn=0 THEN !PRINT "at zero."
12430 !IF Lsn=-1 THEN !PRINT "negative."
12440   REM Extrema values
12450   LET Lst=0
12460   LET Zst=0
12470   FOR I=1 TO Ns
12480     IF Frpx(I)<>0 THEN
12490       LET Tmp=Lsn*ABS(Diel(I))
12500       IF Tmp>Zst OR Zst=0 THEN
12510         LET Zst=Tmp
12520         LET Lst=I
12530       END IF
12540     END IF
12550   NEXT I
12560   IF Lsn=0 THEN Lst=0
12570   LET Alf=CMPLX(0,0)
```

```
12580    IF Lst>0 AND Lst<=Ns+1 THEN
12590       IF Dlog(Lst)<>CMPLX(0,0) THEN Alf=-LOG(Frpx(Lst))/Dlog(Lst)
12600    END IF
12610    LET C0=CMPLX(Lsn,0)
12620    IF Clg2<>CMPLX(0,0) THEN C0=-2*Clg/Clg2!A 2nd guess
12630    LET Wt=ABS(C0)
12640    LET Wt=1/(1+Wt*Wt)!Relative weights for ave the 2 guesses
12650    LET Alf=Alf+Wt*(C0-Alf)!Combined 1st guess
12660    !PRINT "   Guess 1  ";CHR$(224);" = ";
12670    !PRINT DROUND(REAL(Alf),4);DROUND(IMAG(Alf),4)
12680    LET Alf0=CMPLX(0,0)
12690    LET Alferr=1
12700    LET J=2
12710    LET New=0
12720    WHILE Alf<>Alf0 AND J<32 AND Alferr>1.0E-13
12730       IF New=1 THEN
12740          LET Alf0=Alf!Keep track of last iteration
12750          New=0
12760       END IF
12770       LET C1=CMPLX(0,0)
12780       LET C2=CMPLX(0,0)
12790       LET C3=CMPLX(0,0)
12800       LET K=0!Keep count of non-zero terms
12810       FOR I=1 TO Ns
12820          LET C0=Alf*Dlog(I)
12830          IF ABS(REAL(C0))>700 THEN !Failure possible
12840             LET Alf=-2*Clg/Clg2
12850             LET Alf0=CMPLX(0,0)
12860             LET C0=CMPLX(0,0)
12870             LET C1=CMPLX(0,0)
12880             LET Alferr=0!Set to exit
12890          END IF
12900          IF C0<>CMPLX(0,0) AND Diel(I)<>0 THEN
12910             LET C0=Frpx(I)*EXP(C0)
12920             LET C1=C1+C0
12930             LET C2=C2+Dlog(I)*C0
12940             LET C3=C3+Dlog(I)*Dlog(I)*C0
12950             LET K=K+1!Tally another non-zero term
12960          END IF
12970       NEXT I
12980       IF C1<>CMPLX(0,0) AND K>1 THEN ! Log func deriv
12990          REM 0th, 1st, & 2nd logarithmic derivs
13000          LET C2=C2/C1
13010          LET C3=C3/C1-C2*C2
13020          LET C1=LOG(C1)
13030          REM Newton-Raphson estimate via 2nd degree polynomial
13040          LET K1=SGN(REAL(C1))
13050          LET K2=SGN(REAL(C2))
13060          LET C0=CMPLX(0,0)
13070          SELECT K2
13080          CASE 0
13090          !PRINT " o";
13100             IF C3<>CMPLX(0,0) THEN LET C0=-2*C1/C3
13110             IF C0<>CMPLX(0,0) THEN LET Alf=Alf+K1*SQR(C0)
13120          CASE Lsn
```

```
13.30        !PRINT " +";
13140          LET C0=C2*C2-2*C1*C3
13150          IF C0=CMPLX(0,0) THEN
13160            LET C0=2*C1/C2
13170          ELSE
13180            LET C0=2*C1/(C2+K2*SQR(C0))
13190          END IF
13200          LET Alf=Alf-C0    !New estm of exp factor
13210        CASE -Lsn
13220        !PRINT " -";
13230          LET C0=C2*C2-2*C1*C3
13240          IF C0=CMPLX(0,0) THEN
13250            IF C3<>CMPLX(0,0) THEN LET C0=C2/C3
13260          ELSE
13270            IF C3<>CMPLX(0,0) THEN C0=(C2+K2*SQR(C0))/C3
13280          END IF
13290          LET Alf=Alf-C0    !New estm of exp factor
13300        END SELECT
13310        LET Alferr=ABS(REAL(Alf)-REAL(Alf0))+ABS(IMAG(Alf)-IMAG(Alf0))
13320        IF ABS(REAL(Alf))>700 THEN Alf=CMPLX(Lsn/2,0)-Clg/Clg2/(1+J)!Retry
13330        LET New=1                      !Set for update
13340      END IF
13350      !PRINT " Guess";J;" ";CHR$(224);" = ";Alf;" varied¯";Alferr
13360      LET J=J+1
13370    END WHILE
13380    LET Alferr=ABS(Alf0-Alf)    !Iteration variance
13390    !IF Alferr<>0 THEN !PRINT "  Iteration variance =";Alferr
13400    LET Relay(6)=REAL(Alf)      ! Relay the exp ave factor = relay(6&7)
13410    LET Relay(7)=IMAG(Alf)
13420    RETURN Alf
13430 FNEND
13440 !   [    ]    [    ]       SUB Pixs_by_hand     [    ]    [    ]    [    ]
13450 SUB Pixs_by_hand
13460 !***> Subprogram to hand fill a 3D pixel array
13470    COM /Pass/Relay(0:7)
13480    COM /Pixel/ INTEGER Xmax,Ymax,Zmax,Pixl(1:8000),REAL Xscl,Yscl,Zscl
13490    INTEGER Xhnd,Yhnd,Zhnd,Nhnd
13500    FOR Xhnd=1 TO Xmax
13510      FOR Zhnd=Zmax TO 1 STEP -1
13520        FOR Yhnd=1 TO Ymax
13530          LET Nhnd=Xhnd+(Yhnd-1+(Zhnd-1)*Ymax)*Xmax
13540          DISP "Pixl(";VAL$(Xhnd);",";VAL$(Yhnd);",";VAL$(Zhnd);")";
13550          DISP "? (previous=";VAL$(Pixl(Nhnd));")";
13560          INPUT " ",Pixl(Nhnd)
13570        NEXT Yhnd
13580      NEXT Zhnd
13590    NEXT Xhnd
13600 SUBEND
13610 !   [    ]    [    ]    [    ]    [    ]    [    ]    [    ]    [    ]
13620 SUB Pixs_by_random(INTEGER Spclmt)
13630 !***> Subprogram to create a 3D pixel array of random shuffle
13640    COM /Pass/Relay(0:7)
13650    COM /Pixel/ INTEGER Xmax,Ymax,Zmax,Pixl(1:8000),REAL Xscl,Yscl,Zscl
13660    INTEGER Xrdm,Yrdm,Zrdm,Nrdm,Nsf,Spcin,Blks,Seed,Xsf,Ysf,Zsf,Vsf
13670    INTEGER Lsf,Xvr,Yvr,Zvr
```

```
13680    REAL Vrdm,Vtot,Vlm(1:9)
13690    ! Spclmt is integer for max # of species
13700    ! COM /Pass/ uses Relay(0) as vol[1] & Relay(1) seed
13710    !  Relay(2) as random along axis selector
13720    LET Spcin=Spclmt                    !initialize species limit
13730    LET Vtot=0                          !Relative volume accumulator
13740    IF Relay(1)=0 THEN                  !uses Relay(1) as random seed
13750      DISP
13760      INPUT "Random seed? (neg to timer) ",Seed
13770      LET Xsf=1
13780      INPUT "Shuffle along the X direction? 0=no 1=yes (default 1) ",Xsf
13790      IF Xsf<0 THEN STOP
13800      LET Xsf=(Xsf>0)
13810      LET Ysf=1
13820      INPUT "Shuffle along the Y direction? 0=no 1=yes (default 1) ",Ysf
13830      IF Ysf<0 THEN STOP
13840      LET Ysf=(Ysf>0)
13850      LET Zsf=1
13860      INPUT "Shuffle along the Z direction? 0=no 1=yes (default 1) ",Zsf
13870      IF Zsf<0 THEN STOP
13880      LET Zsf=(Zsf>0)
13890    ELSE
13900      LET Seed=INT(.000001+Relay(1))
13910      LET Vsf=INT(.5+Relay(2))         ! Vsf temporary axis selection
13920      LET Xsf=(BIT(Vsf,2)=0)           ! 1,0 for BIT(_,2)=0,1
13930      LET Ysf=(BIT(Vsf,1)=0)           ! 1,0 for BIT(_,1)=0,1
13940      LET Zsf=(BIT(Vsf,0)=0)           ! 1,0 for BIT(_,0)=0,1
13950    END IF
13960    LET Lsf=(Xsf=0 AND Ysf=0 AND Zsf=0) !special case, no shuffling
13970    IF Relay(1)<2 THEN
13980      PRINT "Subprogram ""Pixs_by_random"" fills a pixel box";Xmax;
13990      PRINT "x";Ymax;"x";Zmax;"randomly."
14000      IF Lsf THEN PRINT " NO shuffles, ";
14010      PRINT " Seed=";VAL$(Seed);"; shuffles, X's=";VAL$(Xsf);
14020      PRINT ", Y's=";VAL$(Ysf);", & Z's=";VAL$(Zsf);"."
14030    END IF
14040    LET Xsf=Xsf*(Xmax-1)+1              ! either 1 or Xmax value
14050    LET Ysf=Ysf*(Ymax-1)+1              ! either 1 or Ymax value
14060    LET Zsf=Zsf*(Zmax-1)+1              ! either 1 or Zmax value
14070    LET Vsf=Xsf*Ysf*Zsf                 ! # of elements to shuffle
14080    IF Lsf THEN Vsf=Xmax*Ymax*Zmax
14090    LET Xsf=(Xsf=1)*(Xmax-1)+1          ! either Xmax or 1 value, revrsl
14100    LET Ysf=(Ysf=1)*(Ymax-1)+1          ! either Ymax or 1 value, revrsl
14110    LET Zsf=(Zsf=1)*(Zmax-1)+1          ! either Zmax or 1 value, revrsl
14120    IF Vsf=1 THEN PRINT "TRIVAL Pixl, random shuffling along no direction!"
14130    IF Seed<0 THEN RANDOMIZE TIMEDATE MOD 32767
14140    IF Seed>0 THEN RANDOMIZE Seed
14150    FOR Nrdm=1 TO Spcin
14160      IF Spclmt=Spcin THEN
14170        IF Relay(1)>0 THEN              !use Relay(0) as volume fraction
14180          IF Nrdm=1 THEN LET Vrdm=FRACT(Relay(0))
14190          IF Nrdm=2 THEN LET Vrdm=1-FRACT(Relay(0))
14200          IF Nrdm=3 THEN LET Vrdm=-1
14210        ELSE
14220          DISP "Give occupation for pixel species [";VAL$(Nrdm);"]";
```

```
14230            DISP " of [";VAL$(Spclmt);"]? ";
14240            INPUT "(or <0 ends sequence) ",Vrdm
14250          END IF
14260          IF Vrdm<0 THEN
14270            LET Spclmt=Nrdm-1
14280          ELSE
14290            LET Vtot=Vtot+Vrdm
14300          END IF
14310        END IF
14320        IF Nrdm<=Spclmt THEN
14330          LET Vlm(Nrdm)=Vtot
14340        ELSE
14350          LET Vlm(Nrdm)=0
14360        END IF
14370      NEXT Nrdm
14380      FOR Nrdm=1 TO Spclmt
14390        IF Vtot=0 AND Spclmt>0 THEN
14400          Vlm(Nrdm)=INT(.5+Vsf*Nrdm/Spclmt)
14410        ELSE
14420          Vlm(Nrdm)=INT(.5+Vlm(Nrdm)*Vsf/Vtot)
14430        END IF
14440        !PRINT "v";VAL$(INT(Vlm(Nrdm)));  !debugger
14450      NEXT Nrdm
14460      LET Blks=1                          !keep track of blocks used
14470      FOR Nrdm=1 TO Vsf                   !dispense Pixels as occup. specs
14480        WHILE Nrdm>Vlm(Blks) AND Blks<Spclmt
14490          LET Blks=Blks+1                 !when level exhausted move on
14500        END WHILE
14510        LET Pixl(Nrdm)=Blks
14520      NEXT Nrdm
14530      IF NOT (Lsf) THEN                   !ie, normal shuffling
14540        FOR Nrdm=1 TO Vsf                 !shuffle Pixels
14550          REPEAT
14560            LET Nsf=INT(RND*Vsf)
14570          UNTIL Nsf<>Nrdm AND Nsf<Vsf
14580          LET Blks=Pixl(Nrdm)             !swap
14590          LET Pixl(Nrdm)=Pixl(Nsf+1)
14600          LET Pixl(Nsf+1)=Blks
14610          ! PRINT "s";VAL$(Blks);         !!SHUFFLing sequence,debugger
14620        NEXT Nrdm!!SHUFFLE sequence
14630        ! PRINT
14640        IF NOT (Xsf=1 AND Ysf=1 AND Zsf=1) THEN !if partial, copy out
14650          LET Nsf=Vsf
14660          FOR Zrdm=Zmax TO Zsf STEP -1
14670            FOR Yrdm=Ymax TO Ysf STEP -1
14680              FOR Xrdm=Xmax TO Xsf STEP -1
14690                LET Nrdm=FNOde_mk(Xrdm,Yrdm,Zrdm,Xmax,Ymax,Zmax)
14700                LET Pixl(Nrdm)=Pixl(Nsf)
14710                LET Pixl(Nsf)=0
14720                LET Nsf=Nsf-1
14730              NEXT Xrdm
14740            NEXT Yrdm
14750          NEXT Zrdm
14760        END IF                            ! end if not entire Pixl array
14770        FOR Zrdm=1 TO Zmax
```

```
14780        LET Zvr=Zsf
14790        IF Zvr=1 THEN Zvr=Zrdm
14800        FOR Yrdm=1 TO Ymax
14810          LET Yvr=Ysf
14820          IF Yvr=1 THEN Yvr=Yrdm
14830          FOR Xrdm=1 TO Xmax
14840            Nrdm=FNOde_mk(Xrdm,Yrdm,Zrdm,Xmax,Ymax,Zmax)
14850            LET Xvr=Xsf
14860            IF Xvr=1 THEN LET Xvr=Xrdm
14870            LET Nsf=FNOde_mk(Xvr,Yvr,Zvr,Xmax,Ymax,Zmax)
14880            Pixl(Nrdm)=Pixl(Nsf)
14890          NEXT Xrdm
14900        NEXT Yrdm
14910      NEXT Zrdm
14920    END IF                          !end if, NOT(Lsf)=shuffle OK
14930 SUBEND
14940 !   [    ]   [    ]   [    ]   [    ]   [    ]   [    ]   [    ]
14950 SUB Pixs_by_2block(INTEGER Styps)
14960 !***> Subprogram to create a 3D pixel array of fractal or scaless
14970 !***> grain sizing
14980    COM /Pass/Relay(0:7)
14990    COM /Pixel/ INTEGER Xmax,Ymax,Zmax,Pixl(1:8000),REAL Xscl,Yscl,Zscl
15000    INTEGER Nran,Mran,Nwth,Styp0,Cell,Qnza,Bsz,Jftl,Kftl,Lftl,Nftl,Vftl
15010    INTEGER Aftl,Bftl,Krc,Kqc,Shldr,Xftl,Yftl,Zftl,Xpmx,Ypmx,Zpmx
15020    INTEGER Glv,Myr,Cycl
15030    REAL Vsth,Vall,Vact(1:9)
15040    ! Styps is integer for max # of species, may be changed by SUB
15050    ! COM /Pass/ uses Relay(0) as vol[1] & Relay(1) seed
15060    LET Styp0=Styps                  !initialize species limit
15070    LET Vftl=SHIFT(Xmax,1)*SHIFT(Ymax,1)*SHIFT(Zmax,1) !#2x2x2s
15080    LET Jftl=Xmax*Ymax               !pixels on a Z level
15090    LET Xpmx=Xmax-1                  !next to maximums
15100    LET Ypmx=Ymax-1
15110    LET Zpmx=Zmax-1
15120    LET Nftl=SHIFT(Vftl,1)           !about 50%, 2x2x2s
15130    ALLOCATE INTEGER Sqnc(1:Nftl)    !array of 2x2x2 locations
15140    LET Vall=0                       !Relative volume accumulator
15150    IF Relay(1)=0 THEN               !uses Relay(1) as random seed
15160      DISP
15170      INPUT "Random seed? (neg to timer) ",Qnza
15180    ELSE
15190      LET Qnza=INT(.000001+Relay(1))
15200    END IF
15210    IF Relay(1)<2 THEN
15220      PRINT "Subprogram ""Pixs_by_2block"" fills a pixel box";Xmax;
15230      PRINT "x";Ymax;"x";Zmax;"randomly."
15240      PRINT " shuffle addr: ";
15250    END IF
15260    LET Bsz=Xmax*Ymax*Zmax
15270    IF Nftl<2 OR Vftl=0 THEN         !if Pixl box small
15280      FOR Nran=1 TO Bsz
15290        Pixl(Nran)=BIT(Nran,0)
15300      NEXT Nran
15310      PRINT " Pixel box too small to fractalize, try regular RANDOM"
15320    ELSE
```

```
15330    IF Bsz=1 THEN PRINT "TRIVAL Pixl, random shuffling along no direction!"
15340    IF Qnza<0 THEN RANDOMIZE TIMEDATE MOD 32767
15350    IF Qnza>0 THEN RANDOMIZE Qnza
15360    FOR Nran=1 TO Styp0
15370      IF Styps=Styp0 THEN
15380        IF Relay(1)>0 THEN            !use Relay(0) as volume fraction
15390          IF Nran=1 THEN LET Vsth=FRACT(Relay(0))
15400          IF Nran=2 THEN LET Vsth=1-FRACT(Relay(0))
15410          IF Nran=3 THEN LET Vsth=-1
15420        ELSE
15430          DISP "Give occupation for pixel species [";VAL$(Nran);"]";
15440          DISP " of [";VAL$(Styps);"]? ";
15450          INPUT "(or <0 ends sequence) ",Vsth
15460        END IF
15470        IF Vsth<0 THEN
15480          LET Styps=Nran-1
15490        ELSE
15500          LET Vall=Vall+Vsth
15510        END IF
15520      END IF
15530      IF Nran<=Styps THEN
15540        LET Vact(Nran)=Vall
15550      ELSE
15560        LET Vact(Nran)=0
15570      END IF
15580    NEXT Nran
15590    FOR Nran=1 TO Styps
15600      IF Vall=0 AND Styps>0 THEN
15610        Vact(Nran)=INT(.5+Bsz*Nran/Styps)
15620      ELSE
15630        Vact(Nran)=INT(.5+Vact(Nran)*Bsz/Vall)
15640      END IF
15650    !PRINT "v";VAL$(INT(Vact(Nran))); !debugger
15660    NEXT Nran
15670    LET Cell=1                        !keep track of blocks used
15680    LET Kftl=0                        ! count Pixl=[1]s
15690    FOR Nran=1 TO Bsz                 !dispense Pixels as occup. specs
15700      WHILE Nran>Vact(Cell) AND Cell<Styps
15710        LET Cell=Cell+1               !when level exhausted move on
15720      END WHILE
15730      LET Pixl(Nran)=Cell
15740      IF Cell=1 THEN Kftl=Kftl+1      ! increment count of Pixl=[1]s
15750    NEXT Nran
15760    FOR Nran=1 TO Nftl               ! make 2x2x2 locations
15770      REPEAT
15780        LET Shldr=1
15790        REPEAT                        ! get randomly X up to Xmax-1, etc
15800          LET Xftl=INT(RND*Xpmx)
15810        UNTIL Xftl<Xpmx
15820        REPEAT
15830          LET Yftl=INT(RND*Ypmx)
15840        UNTIL Yftl<Ypmx
15850        REPEAT
15860          LET Zftl=INT(RND*Zpmx)
15870        UNTIL Zftl<Zpmx
```

```
15880          LET Nwth=1+Xftl+Yftl*Xmax+Zftl*Jftl !formulate Pixl address
15890          FOR Mran=1 TO Nran-1        ! check if good new address
15900            LET Aftl=Nwth-Sqnc(Mran) ! address differences
15910            IF Aftl=0 THEN           ! at same location
15920              LET Shldr=0
15930            ELSE                      ! or neighbor checking
15940              LET Zftl=ABS(Aftl DIV Jftl)
15950              LET Xftl=ABS(Aftl MOD Jftl)
15960              LET Yftl=ABS(Xftl DIV Xmax)
15970              LET Xftl=ABS(Xftl MOD Xmax)
15980              LET Bftl=(Xftl>1 OR Yftl>1 OR Zftl>1) !test, not overlap
15990              !PRINT VAL$(Bftl);
16000              IF NOT Bftl THEN Shldr=0
16010            END IF                    !endif, neighbor checking, Aftl
16020          NEXT Mran                   !next checking in sequence
16030          IF Shldr THEN Sqnc(Nran)=Nwth !assign another 2x2x2
16040        UNTIL Shldr
16050      NEXT Nran
16060      FOR Nran=1 TO Nftl-1            !shuffle 2x2x2s
16070        LET Mran=Sqnc(Nran)          !randomly exchange in sequence
16080        REPEAT                        !with another higher up
16090          LET Nwth=INT(RND*(Nftl-Nran))
16100        UNTIL Nwth<(Nftl-Nran)
16110        LET Nwth=Sqnc(Nwth+Nran+1)
16120        IF Relay(1)<2 THEN PRINT Mran;"<=>";Nwth;";"; !exchange details
16130        FOR Krc=0 TO 7                !range thru Pixls in 2x2x2s
16140          LET Aftl=BIT(Krc,2)+BIT(Krc,1)*Xmax+BIT(Krc,0)*Jftl
16150          LET Cell=Pixl(Mran+Aftl)
16160          LET Pixl(Mran+Aftl)=Pixl(Nwth+Aftl)
16170          LET Pixl(Nwth+Aftl)=Cell
16180        NEXT Krc
16190      NEXT Nran
16200      IF Relay(1)<2 THEN PRINT
16210      FOR Nran=1 TO Nftl             ! add random orientations
16220        LET Mran=Sqnc(Nran)
16230        REPEAT                        ! get a random #
16240          LET Krc=INT(RND*16)
16250        UNTIL Krc<16
16260        LET Kqc=SHIFT(Krc,2)          ! 0=none 1<>Xs 2<>Ys 3<>Zs
16270        IF Kqc>0 THEN                 ! Kqc>0 >=> random exchanges
16280          FOR Glv=0 TO 1              ! do 2 levels the same
16290            FOR Myr=0 TO BIT(Krc,1)   ! 0=diag 1=flatwise (2 passes)
16300              LET Xftl=Glv            ! 1st exchange relv coordinates
16310              LET Yftl=Myr
16320              LET Zftl=BIT(Krc,0)
16330              IF Myr THEN Zftl= NOT Zftl! reverse 2nd pass of Myr
16340              FOR Cycl=2 TO Kqc       ! cyclic permutation
16350                LET Cell=Zftl
16360                LET Zftl=Yftl
16370                LET Yftl=Xftl
16380                LET Xftl=Cell
16390              NEXT Cycl
16400              LET Aftl=1+Xftl+Yftl*Xmax+Zftl*Jftl
16410              !PRINT " <";VAL$(Mran);">(";VAL$(Xftl);",";VAL$(Yftl);",";
16420              !PRINT VAL$(Zftl);")< >";
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16430              LET Xftl=Glv            ! 2nd exchange coordinates
16440              LET Yftl=Myr            ! same as 1st but add NOTs
16450              LET Zftl=BIT(Krc,0)
16460              IF Myr THEN Zftl= NOT Zftl! reverse upon 2nd pass
16470              IF BIT(Krc,0)=0 OR BIT(Krc,1)=0 THEN Yftl= NOT Yftl
16480              IF BIT(Krc,0)=1 OR BIT(Krc,1)=0 THEN Zftl= NOT Zftl
16490              FOR Cycl=2 TO Kqc       ! cyclic permutation
16500                 LET Cell=Zftl
16510                 LET Zftl=Yftl
16520                 LET Yftl=Xftl
16530                 LET Xftl=Cell
16540              NEXT Cycl
16550              LET Bftl=1+Xftl+Yftl*Xmax+Zftl*Jftl
16560              !PRINT "(";VAL$(Xftl);",";VAL$(Yftl);",";VAL$(Zftl);")";
16570              LET Cell=Pixl(Mran+Aftl)! swap
16580              LET Pixl(Mran+Aftl)=Pixl(Mran+Bftl)
16590              LET Pixl(Mran+Bftl)=Cell
16600           NEXT Myr
16610         NEXT Glv
16620       END IF                          ! endif, Kqc>0, random exchanges
16630       FOR Krc=0 TO 7                   ! tag the large blocks
16640         LET Aftl=1+BIT(Krc,2)+BIT(Krc,1)*Xmax+BIT(Krc,0)*Jftl
16650         LET Pixl(Mran+Aftl)=BINCMP(Pixl(Mran+Aftl))
16660       NEXT Krc
16670     NEXT Nran
16680     IF (Bsz-SHIFT(Nftl,-3))>2 THEN ! shuffle rest unmarked
16690       FOR Nran=1 TO Bsz
16700         IF Pixl(Nran)>=0 THEN
16710           REPEAT
16720             LET Mran=Bsz*RND
16730             IF Mran<Bsz THEN          ! test for Pixl marked/unmarked
16740               LET Myr=Pixl(Mran+1)
16750             ELSE
16760               LET Myr=-1
16770             END IF
16780           UNTIL Mran<>Nran AND Myr>=0
16790           LET Mran=Mran+1
16800           LET Cell=Pixl(Nran)         ! swap
16810           LET Pixl(Nran)=Pixl(Mran)
16820           LET Pixl(Mran)=Cell
16830         END IF                        ! end if, Pixl test
16840       NEXT Nran
16850     END IF                            ! end if, shuffle unmarked
16860     LET Cell=0                        ! start to count Pixl=[1]s
16870     FOR Nran=1 TO Bsz                 ! remove marking
16880       IF Pixl(Nran)<0 THEN Pixl(Nran)=BINCMP(Pixl(Nran))
16890       IF Pixl(Nran)=1 THEN Cell=Cell+1
16900     NEXT Nran
16910     IF Cell<>Kftl THEN PRINT " Lost/gained something in SUB shuffle"
16920     !PRINT
16930     !PRINT Sqnc(*)
16940     DEALLOCATE Sqnc(*)
16950   END IF                              !end if, for big enuf Pixl box
16960 SUBEND
16970 !     [     ]     [     ]     [     ]     [     ]     [     ]     [     ]
```

```
16980 SUB Pixs_by_ellps
16990    COM /Pass/Relay(0:7)
17000    COM /Pixel/ INTEGER Xmax,Ymax,Zmax,Pixl(1:8000),REAL Xscl,Yscl,Zscl
17010    !***> Creates a 3D pixel array of an ellisoidal inclusion in a host
17020    INTEGER Blkc1,Blkc2,Boxz,Btst,Dsr,Impv,Roll,Tally,Uyou,Xlv,Ylv,Zlv
17030    REAL Chgu,Flvr,Frs1,Frs2,Guess
17040    REAL Xgu,Ygu,Zgu,Vlps,Xlps,Ylps,Zlps,Xflv,Yflv
17050    LET Boxz=Xmax*Ymax*Zmax
17060    IF Boxz<=0 THEN PRINT Xmax;"x";Ymax;"x";Zmax;"??? .n SUB ellps"
17070    LET Uyou=(Relay(0)=0)                !user input signal
17080    IF Uyou THEN
17090      DISP
17100      PRINT "Filling pixels with ellipsoid inclusion imbedded in";
17110      PRINT " a host (a binary)"
17120      LET Frs1=1
17130      IF Relay(0)>0 THEN Frs1=Relay(0)
17140      DISP "Give occupation by species [1]? (default=";VAL$(Frs1);
17150      INPUT ") ",Frs1
17160      LET Frs2=1
17170      IF Frs1>0 AND Frs1<1 THEN Frs2=1-Frs1
17180      DISP "Give occupation by species [2]? (default=";VAL$(Frs2);
17190      INPUT ") ",Frs2
17200      DISP "Inclusion role? 0)=smaller species, 1)=species #1,";
17210      INPUT " 2)=species #2 ",Roll
17220      IF Roll<0 THEN STOP
17230      LET Xlps=1
17240      INPUT "Ellipsoid X axis length? (default=1) ",Xlps
17250      LET Ylps=1
17260      INPUT "Ellipsoid Y axis length? (default=1) ",Ylps
17270      LET Zlps=1
17280      INPUT "Ellipsoid Z axis length? (default=1) ",Zlps
17290      PRINT "Subprogram ""Pixs_by_ellps"" fills a pixel box";Xmax;
17300      PRINT "x";Ymax;"x";Zmax;"with an ellipsiod"
17310    ELSE
17320      LET Frs1=FRACT(Relay(0))         !Relay(0)=volume fraction of [1]
17330      LET Frs2=1-Frs1
17340      LET Roll=(Relay(4)>.5)           !Relay(4) is role reversal flag
17350      LET Xlps=Relay(1)                !Relay(1) is X ellipse axis
17360      LET Ylps=Relay(2)                !Relay(2) is Y ellipse axis
17370      LET Zlps=Relay(3)                !Relay(3) is Z ellipse axis
17380    END IF                             !end if,Uyou
17390    IF Roll>2 THEN LET Roll=2-BIT(Roll,0)
17400    LET Frs2=Frs1+Frs2
17410    IF Frs2>0 THEN Frs1=Frs1/Frs2      !Normalize fractions
17420    LET Frs2=1-Frs1
17430    IF Roll=0 THEN Roll=1+(Frs1>.5)    !program selects inclusion role
17440    IF Roll=1 THEN Dsr=INT(.5+Boxz*Frs1)
17450    IF Roll=2 THEN Dsr=INT(.5+Boxz*Frs2)
17460    IF Xlps<=0 THEN Xlps=1
17470    IF Ylps<=0 THEN Ylps=1
17480    IF Zlps<=0 THEN Zlps=1
17490    LET Vlps=.5*PI*Xlps*Ylps*Zlps      !3*ellipse quandrant user size param
17500    LET Impv=0
17510    LET Guess=(3*Dsr/Vlps)^(1/3)       !initial guess at axis scaling factor
17520    LET Blkc1=SHIFT(-1,1)              !assume worst case to start,MAXINT
```

```
17530    LET Blkc2=SHIFT(-1,1)                !assume worst case to start,MAXINT
17540    LET Impv=4                          !least 3 guesses
17550    REPEAT                              !until guess improved
17560      LET Impv=Impv-1
17570      LET Xgu=Guess*Xlps
17580      LET Ygu=Guess*Ylps
17590      LET Zgu=Guess*Zlps
17600      LET Xgu=Xgu*Xgu
17610      LET Ygu=Ygu*Ygu
17620      LET Zgu=Zgu*Zgu
17630      LET Tally=0
17640      FOR Xlv=1 TO Xmax
17650        LET Xflv=((.5+Xlv)*(.5+Xlv))/Xgu
17660        FOR Ylv=1 TO Ymax
17670          LET Yflv=((.5+Ylv)*(.5+Ylv))/Ygu
17680          FOR Zlv=1 TO Zmax
17690            LET Flvr=((.5+Zlv)*(.5+Zlv))/Zgu+Xflv+Yflv
17700            LET Tally=Tally+(Flvr<=1) !Tally pixels within ellipsoid
17710          NEXT Zlv
17720        NEXT Ylv
17730      NEXT Xlv
17740      LET Btst=Tally-Dsr                 !How far off the mark is the Tally
17750      !PRINT "c";VAL$(Btst);
17760      IF Btst<0 THEN
17770        IF -Btst<Blkc1 THEN              !new lower minumum found
17780          LET Blkc1=-Btst
17790          LET Impv=3
17800        END IF
17810      END IF
17820      IF Btst>0 THEN                     !new upper maximum found
17830        IF Btst<Blkc2 THEN
17840          LET Blkc2=Btst
17850          LET Impv=3
17860        END IF
17870      END IF
17880      LET Chgu=Btst/(Guess*Guess*Vlps)  !estimate correction to guess
17890      IF Impv>0 THEN Guess=Guess-Chgu
17900      IF Guess<=0 AND Impv>0 THEN Guess=(Guess+Chgu)*.5
17910    UNTIL Impv<=0                        !until nolonger improves
17920    !PRINT
17930    IF Guess<>0 THEN
17940      IF Guess<0 THEN Guess=-Guess
17950      FOR Xlv=1 TO Xmax
17960        LET Xflv=((.5+Xlv)*(.5+Xlv))/Xgu
17970        FOR Ylv=1 TO Ymax               !assign Pixls
17980          LET Yflv=((.5+Ylv)*(.5+Ylv))/Ygu
17990          FOR Zlv=1 TO Zmax
18000            LET Flvr=((.5+Zlv)*(.5+Zlv))/Zgu+Xflv+Yflv
18010            LET Tally=Xlv+(Ylv-1+(Zlv-1)*Ymax)*Xmax
18020            IF Roll=1 THEN LET Pixl(Tally)=1+(Flvr>1)
18030            IF Roll=2 THEN LET Pixl(Tally)=2-(Flvr>1)
18040          NEXT Zlv
18050        NEXT Ylv
18060      NEXT Xlv
18070      IF Uyou THEN
```

```
18080          PRINT " whose size is: X axis=";VAL$(DROUND(Xlps*Guess,4));
18090          PRINT ", Y axis=";VAL$(DROUND(Ylps*Guess,4));
18100          PRINT ", & Z axis=";VAL$(DROUND(Zlps*Guess,4));"."
18110        END IF
18120     END IF                              !end if guess<>0
18130  SUBEND
18140  SUB Pix_by_correlat
18150     COM /Pass/Relay(0:7)
18160     COM /Pixel/ INTEGER Xmax,Ymax,Zmax,Pixl(1:8000),REAL Xscl,Yscl,Zscl
18170     INTEGER Bcrl,Crrl,Gcrl,Icrl,Jcrl,Kcrl,Lcrl,Ncrl,Qcrl,Scrl,Tcrl,Zcrl
18180     INTEGER Xc,Yc,Zc,Xdf,Ydf,Zdf
18190     REAL Arel,Prel,Rrel,Vrel,Vsm,Frel(1:9)
18200     LET Zcrl=Xmax*Ymax                   ! Pixel box area of Z section
18210     LET Bcrl=Zcrl*Zmax                   ! Total max Pixels
18220     ALLOCATE Tabl(1:Bcrl),Wrel(0:Bcrl)   ! For correlation weighting
18230     MAT Pixl=(0)                         ! Need to zero out pixels
18240     LET Vsm=0                            ! Volume fraction
18250     LET Crrl=INT(Relay(2))               ! Pass correlation selection
18260     IF Crrl=1 OR Crrl=4 THEN Prel=Relay(3) ! Pass correlation length
18270     IF Relay(1)=0 THEN
18280        DISP
18290        INPUT "Random seed? (negative to timer)",Scrl
18300        DISP "Correlation? none=0 expon=1 inverse=2 inv square=3";
18310        DISP " power law=4 (default=";VAL$(Crrl);
18320        INPUT ")",Crrl
18330        LET Relay(2)=Crrl
18340     ELSE
18350        LET Scrl=(.00000000001+Relay(1))
18360     END IF
18370     IF Scrl>0 THEN RANDOMIZE Scrl        ! Seeding random generator
18380     IF Scrl<0 THEN RANDOMIZE TIMEDATE MOD 32767
18390     LET Vrel=(Xmax-1)*(Xmax-1)+(Ymax-1)*(Ymax-1)+(Zmax-1)*(Zmax-1)
18400      !LET Vrel=Xmax*Xmax+Ymax*Ymax+Zmax*Zmax ! =hypotenuse diag squared
18410     SELECT Crrl
18420     CASE =1                              ! exponential correlation
18430        IF Relay(1)=0 THEN
18440           DISP "Correlation length? (in pixel units, default=";
18450           DISP VAL$(Prel);
18460           INPUT ")",Prel
18470        END IF
18480        IF Prel=0 THEN Prel=SQR(Vrel)*.5   ! if zero, then .5 diag
18490        LET Relay(3)=Prel
18500        LET Arel=EXP(SQR(Vrel)/Prel)      ! field weighting factor
18510     CASE =2                              ! inverse correlation
18520        LET Arel=SQR(Vrel)
18530     CASE =3                              ! inverse square correlation
18540        LET Arel=Vrel
18550     CASE =4                              ! power law correlation
18560        IF Relay(1)=0 THEN
18570           DISP "Power law? (1=inverse, 2=inv sqr, etc, default=";
18580           DISP VAL$(Prel);
18590           INPUT ")",Prel
18600           LET Relay(3)=Prel
18610        END IF
18620        IF Prel=0 THEN
```

```
18630          LET Crrl=0
18640        ELSE
18650          LET Arel=Vrel^(Prel*.5)
18660        END IF
18670      CASE ELSE
18680        LET Arel=1
18690      END SELECT
18700      LET Tcrl=0                         ! Species tally
18710      FOR Ncrl=1 TO 9                    ! up to 9 species
18720        LET Frel(Ncrl)=0
18730        IF Tcrl=0 THEN                   ! Has not ended sequence
18740          IF Relay(1)>0 THEN            ! get next occupation
18750            IF Ncrl=1 THEN Vrel=FRACT(Relay(0))
18760            IF Ncrl=2 THEN Vrel=1-FRACT(Relay(0))
18770            IF Ncrl=3 THEN Vrel=-1
18780          ELSE                           ! manual operation
18790            DISP "Give occupation for species [";VAL$(Ncrl);
18800            INPUT "] or (<0 ends sequence)",Vrel
18810          END IF
18820          IF Vrel<0 THEN
18830            LET Tcrl=Ncrl-1              ! # of species at sequence end
18840            LET Frel(Ncrl)=0
18850          ELSE
18860            LET Vsm=Vsm+Vrel
18870            LET Frel(Ncrl)=Vsm          ! Accumulative volume
18880          END IF
18890        END IF
18900      NEXT Ncrl
18910      IF Vsm<>0 THEN LET Vsm=Bcrl/Vsm    ! Normalize to Pixel allotment
18920      FOR Ncrl=1 TO Tcrl                 ! Intergerize up to Bcrl total
18930        IF Frel(Ncrl)<>0 THEN Frel(Ncrl)=INT(Frel(Ncrl)*Vsm+.5)
18940        IF Vsm=0 THEN Frel(Ncrl)=INT(Ncrl*Bcrl/Tcrl+.5)
18950      NEXT Ncrl
18960      FOR Ncrl=Tcrl TO 2 STEP -1         ! Convert to allotments
18970        LET Frel(Ncrl)=INT(Frel(Ncrl)-Frel(Ncrl-1)+.5)
18980      NEXT Ncrl
18990      LET Vsm=SUM(Frel)
19000      IF Vsm<>Bcrl THEN PRINT "Unable to place all pixels, see SUB"
19010      IF Relay(1)=0 THEN
19020        PRINT " pixs allocations, sum=";VAL$(Vsm);" @";
19030        PRINT Frel(*);
19040        PRINT
19050      END IF
19060      LET Xc=0                           ! Initialize addresses
19070      LET Yc=1
19080      LET Zc=1
19090      FOR Ncrl=1 TO Bcrl                 ! Set up weights tabulation
19100        LET Xc=Xc+1                      ! to avoid excessive recomputations
19110        IF Xc>Xmax THEN
19120          LET Xc=1
19130          LET Yc=Yc+1
19140          IF Yc>Ymax THEN
19150            LET Yc=1
19160            LET Zc=Zc+1
19170          END IF
```

```
19180      END IF
19190      LET Vrel=(Xc-1)*(Xc-1)+(Yc-1)*(Yc-1)+(Zc-1)*(Zc-1) ! sep distance
19200      SELECT Crrl                         ! select correlation potentials
19210      CASE =0
19220        LET Vrel=1
19230      CASE =1
19240        LET Vrel=EXP(SQR(Vrel)/Prel)
19250      CASE =2
19260        IF Vrel<>0 THEN Vrel=SQR(Vrel)
19270      CASE =4
19280        IF Vrel<>0 THEN Vrel=Vrel^(Prel*.5)
19290      END SELECT
19300      IF Vrel=0 THEN
19310        LET Tabl(Ncrl)=0
19320      ELSE
19330        LET Tabl(Ncrl)=Arel/Vrel
19340      END IF
19350      NEXT Ncrl
19360      IF Relay(1)=0 THEN                  ! correlation potentials map
19370        FOR Xc=1 TO Xmax
19380          PRINT "X-section weight to origin, plane =";Xc
19390          FOR Zc=Zmax TO 1 STEP -1
19400            FOR Yc=1 TO Ymax
19410              LET Ncrl=Xc+(Yc-1)*Xmax+(Zc-1)*Zcrl
19420              PRINT USING """|"".7A,#";VAL$(DROUND(Tabl(Ncrl),3))
19430            NEXT Yc
19440            PRINT
19450          NEXT Zc
19460        NEXT Xc
19470      END IF                              ! end if, map
19480      REM  Finding the weighting field . . . . . . . . . >
19490      PRINT "  Wait filling";Bcrl;"Pixels in SUB Pix_by_correlat"
19500      LET Rrel=RND                        ! prime the RND generator
19510      FOR Icrl=Bcrl TO 1 STEP -1          ! Roam thru random fill positions
19520        LET Kcrl=0
19530        LET Gcrl=0
19540        FOR Jcrl=1 TO Tcrl                ! Fill random ordering sequence
19550          IF INT(Frel(Jcrl))>.5 THEN
19560            LET Kcrl=Kcrl+INT(Frel(Jcrl)+.5) ! summation of remaining to fill
19570            LET Gcrl=Gcrl+1               ! tally of remaining pixel species
19580          END IF
19590        NEXT Jcrl
19600        IF Gcrl>1 THEN                    ! Fill randomly,>1 pixels to fill
19610          REPEAT
19620            LET Ncrl=INT(RND*Kcrl)        ! get random #
19630          UNTIL Ncrl<Kcrl
19640          LET Ncrl=Ncrl+1
19650          LET Lcrl=0
19660          LET Kcrl=0
19670          FOR Jcrl=1 TO Tcrl
19680            IF Frel(Jcrl)>.5 AND Lcrl=0 THEN
19690              LET Kcrl=Kcrl+INT(Frel(Jcrl)+.5)
19700              IF Kcrl>=Ncrl THEN          ! contains address of non-zero
19710                LET Lcrl=Jcrl
19720                LET Frel(Lcrl)=Frel(Lcrl)-1! reduce one more
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19730           END IF
19740         END IF
19750       NEXT Jcrl
19760       PRINT "[";VAL$(Lcrl);"]";
19770       MAT Wrel=(0)
19780       LET Kcrl=0
19790       FOR Jcrl=1 TO Bcrl              ! Find pixel weighting field
19800         LET Zc=(Jcrl-1) DIV Zcrl
19810         LET Xc=(Jcrl-1) MOD Zcrl
19820         LET Yc=Xc DIV Xmax
19830         LET Xc=Xc MOD Xmax
19840         IF Pixl(Jcrl)=0 THEN          ! for unfilled or zeroed pixels
19850           LET Kcrl=Kcrl+1
19860           FOR Ncrl=1 TO Bcrl
19870             IF Pixl(Ncrl)=Lcrl THEN ! This pixel contributes to weighting
19880               LET Zdf=ABS(((Ncrl-1) DIV Zcrl)-Zc)
19890               LET Qcrl=(Ncrl-1) MOD Zcrl
19900               LET Ydf=ABS((Qcrl DIV Xmax)-Yc)
19910               LET Xdf=ABS((Qcrl MOD Xmax)-Xc)
19920               LET Qcrl=1+Xdf+Ydf*Xmax+Zdf*Zcrl! for tabulation address
19930               !LET Vrel=Xdf*Xdf+Ydf*Ydf+Zdf*Zdf !Square of rel diff in addr
19940               IF Qcrl>0 THEN Wrel(Kcrl)=Wrel(Kcrl)+Tabl(Qcrl)
19950             END IF                   ! end if, Pixl=Lcrl test
19960           NEXT Ncrl
19970         END IF                       ! end if, Pixl=0 test
19980       NEXT Jcrl
19990       LET Vsm=0
20000       FOR Jcrl=1 TO Kcrl             ! total of weighting
20010         LET Vsm=Vsm+Wrel(Jcrl)
20020       NEXT Jcrl
20030       IF Vsm<=0 THEN
20040         FOR Jcrl=1 TO Kcrl
20050           LET Wrel(Jcrl)=1
20060         NEXT Jcrl
20070         LET Vsm=Kcrl
20080         PRINT "e";
20090       END IF
20100 !     IF Icrl<Bcrl-3 AND Icrl>Bcrl-5 THEN ! Set for intermediate printout
20110 !       PRINT
20120 !       PRINT " Weighting map at fill #";VAL$(Bcrl-Icrl+1);":"
20130 !       FOR Zdf=1 TO Zmax
20140 !         PRINT " Pixels in Z-sectional plane";Zdf;
20150 !         PRINT "(interaction to [";VAL$(Lcrl);"])"
20160 !         FOR Ydf=1 TO Ymax
20170 !           LET Jcrl=(Ydf-1)*Xmax+(Zdf-1)*Zcrl
20180 !           FOR Xdf=1 TO Xmax
20190 !             LET Qcrl=Jcrl+Xdf
20200 !             PRINT USING "2X,""["",A,""]"",3X,#";VAL$(Pixl(Qcrl))
20210 !           NEXT Xdf
20220 !           PRINT
20230 !         NEXT Ydf
20240 !       NEXT Zdf
20250 !       LET Qcrl=0
20260 !       LET Zdf=0
20270 !       FOR Jcrl=1 TO Bcrl
```

```
20280 !          IF (Jcrl-1) MOD Zcrl=0 THEN
20290 !            LET Zdf=Zdf+1
20300 !            PRINT "Weights in Z plane";Zdf
20310 !          END IF
20320 !          IF Pixl(Jcrl)=0 THEN
20330 !            LET Qcrl=Qcrl+1
20340 !            PRINT USING """"|"",7A,#";VAL$(INT(Wrel(Qcrl)+.5))
20350 !          ELSE
20360 !            PRINT "|none   ";
20370 !          END IF
20380 !          IF Jcrl MOD Xmax=0 THEN PRINT
20390 !        NEXT Jcrl
20400 !      END IF                        ! end if, intermediate printout
20410       REPEAT                         ! Get a RANDOM #
20420         LET Rrel=RND*Vsm
20430       UNTIL Rrel<Vsm
20440       LET Qcrl=1                     ! Testing switch is set to ON
20450       LET Kcrl=0                     ! Keep tally of Pixels with zeros
20460       LET Vsm=0                      ! Zero weighting accumulator
20470       FOR Jcrl=1 TO Bcrl
20480         IF Qcrl AND Pixl(Jcrl)=0 THEN ! Test if Pixel is zero
20490           LET Kcrl=Kcrl+1            ! Further assign if = RANDOM #
20500           LET Vsm=Vsm+Wrel(Kcrl)     ! Accumalative weight
20510           IF Vsm>Rrel THEN           ! Trips when reach RANDOM #
20520             LET Pixl(Jcrl)=Lcrl      ! Pixel assigned
20530             LET Qcrl=0               ! No more testing set
20540           END IF
20550         END IF                       ! end if, Pixl=0 test
20560       NEXT Jcrl
20570     ELSE                             ! Only 0 OR 1 TYPES, fast fill
20580       LET Lcrl=0
20590       FOR Jcrl=1 TO Tcrl
20600         IF Frel(Jcrl)<>0 THEN Lcrl=Jcrl
20610       NEXT Jcrl
20620       IF Lcrl>0 THEN
20630         FOR Jcrl=1 TO Bcrl           ! filling the remaining, 1 type
20640           IF Pixl(Jcrl)=0 THEN
20650             LET Pixl(Jcrl)=Lcrl
20660             LET Frel(Lcrl)=Frel(Lcrl)-1
20670           END IF
20680         NEXT Jcrl
20690       END IF
20700     END IF                           ! end if, Gcrl>1 test
20710   NEXT Icrl
20720   IF Relay(1)=0 THEN PRINT "&";SUM(Frel);"remain."
20730   DEALLOCATE Tabl(*),Wrel(*)         ! Bye-bye variable sub arrays
20740 SUBEND
20750 SUB Pixs_by_evolv(INTEGER Gpcs)
20760   COM /Pass/Relay(0:7)
20770   COM /Pixel/ INTEGER Xmax,Ymax,Zmax,Pixl(1:8000),REAL Xscl,Yscl,Zscl
20780   INTEGER Cnk,Clmx,Gens,Shv,Fadr,Rlr,Mdl,Mlk1,Mlk2,Nsft,Rset,Sadr,Vlv
20790   INTEGER Gski,Kski,Mski,Qski,Sski,Xski,Yski,Zski,Ncs(0:9),Pcs(0:9)
20800   REAL Agen,Dv,Prpt,Vski,Dmd(0:9)
20810   LET Cnk=Xmax*Ymax*Zmax
20820   FOR Sski=1 TO Cnk
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```
20830       LET Pixl(Sski)=0                    ! Need to zero out pixels
20840   NEXT Sski
20850   LET Vski=0                              ! Volume fraction
20860   LET Mski=(Relay(1)=0)                   ! manual indicator
20870   LET Rset=Relay(2)                       ! Pass vols preservation
20880   LET Rset=BIT(Rset,0)
20890   LET Gens=Relay(3)                       ! Pass generation size
20900   LET Vlv=Relay(4)                        ! Evolution starter
20910   LET Prpt=FRACT(Relay(5))                ! proportion change
20920   IF Gpcs=0 THEN Gpcs=2                    ! default to binary
20930   IF Mski THEN
20940     DISP
20950     INPUT "Random seed? (negative to timer, none=0)",Shv
20960     IF Shv=0 THEN                          ! From generation to generation
20970       LET Rset=1                           ! preserve vol fractions
20980     ELSE
20990       DISP "Maintain constant parent to descendent";
21000       DISP " ratios? Vary=0 Fixed=1 (default=";VAL$(Rset);
21010       INPUT ")",Rset
21020       LET Rset=BIT(Rset,0)
21030       LET Relay(2)=Rset
21040     END IF
21050     DISP "Generations of evolution? (self determine=0, default=";Gens;
21060     INPUT ")",Gens
21070     LET Relay(3)=Gens
21080   ELSE                                     ! get parameters from Relays
21090     LET Shv=Relay(1)                       ! seed
21100     IF Shv=0 THEN
21110       LET Rset=1
21120     ELSE
21130       LET Gpcs=2
21140       Dmd(1)=FRACT(Relay(0))
21150       Dmd(2)=1-Dmd(1)
21160     END IF
21170   END IF                                   ! end if, relays
21180   IF Gens=0 THEN
21190     LET Agen=MAX(Xmax,Ymax,Zmax)          ! set Gens upward integer
21200     LET Gens=-INT(1-LOG(Agen)/LOG(2.0))
21210   END IF
21220   IF Gens<0 THEN STOP
21230   IF Gens=0 THEN PRINT "No evolutions?"
21240   LET Qski=7                               ! elements per expansion cube
21250   LET Mlk1=Xmax                            ! set multipiers for addresses
21260   IF Xmax=1 THEN Mlk1=Ymax
21270   LET Mlk2=Xmax*Ymax
21280   IF Xmax=1 THEN LET Qski=SHIFT(Qski,1)
21290   IF Ymax=1 THEN LET Qski=SHIFT(Qski,1)
21300   IF Zmax=1 THEN LET Qski=SHIFT(Qski,1)
21310   LET Clmx=Qski+1
21320   ALLOCATE REAL Ruls(0:Gpcs,0:9)
21330   IF Shv>0 THEN RANDOMIZE Shv              ! Seeding random generator
21340   IF Shv<0 THEN RANDOMIZE TIMEDATE MOD 32767
21350   IF Mski THEN
21360     PRINT " ";Gens;"generations could expand to fill a cube sized";
21370     LET Agen=(2.0)^(Gens+1.0)             ! Pixel cube edge
```

```
21380      PRINT " ";VAL$(Agen);"x";VAL$(Agen);"x";VAL$(Agen);"."
21390    END IF
21400    IF Shv=0 THEN                         ! generate pattern fills
21410      FOR Gski=1 TO Gpcs                  ! up to 9 species
21420        FOR Sski=0 TO Qski                ! bit ordering of Sski is (Z,Y,X)s
21430          LET Ruls(Gski,Sski)=Gski     ! default
21440          DISP "Evolution from parent species [";VAL$(Gski);
21450          DISP "], sector (";VAL$(BIT(Sski,0));
21460          IF Qski>1 THEN DISP ",";VAL$(BIT(Sski,1));
21470          IF Qski>3 THEN DISP ",";VAL$(BIT(Sski,2));
21480          DISP ") is to species? (default=[";VAL$(Gski);
21490          INPUT "])",Ruls(Gski,Sski)
21500          LET Ruls(Gski,Sski)=INT(.5+Ruls(Gski,Sski))
21510        NEXT Sski
21520      NEXT Gski
21530    ELSE
21540      IF Rset=1 THEN                      ! get shuffle fills
21550        FOR Gski=1 TO Gpcs
21560          LET Mdl=0
21570          LET Kski=0
21580          FOR Sski=Clmx TO 1 STEP -1
21590            WHILE Mdl<1 AND Kski<=Gpcs
21600              LET Kski=Kski+1             ! current species fill
21610              IF Mski THEN
21620                DISP "How many descendants for species [";VAL$(Kski);
21630                DISP "] evolve from parent species [";VAL$(Gski);"]";
21640                DISP " (up to ";VAL$(Sski);
21650                INPUT ")",Mdl
21660              ELSE
21670                IF Kski=Gski THEN
21680                  LET Mdl=(1-Prpt)*Qski+.5
21690                ELSE
21700                  LET Mdl=Prpt*Qski
21710                END IF
21720              END IF                      ! endif, Mski=0 test
21730            END WHILE                     ! endif, Mdl<1 test
21740            LET Ruls(Gski,Clmx-Sski)=Kski
21750            LET Mdl=Mdl-1
21760          NEXT Sski
21770        NEXT Gski
21780      ELSE                                ! else, fill by demands
21790        LET Ruls(0,0)=0
21800        LET Nsft=0
21810        IF Mski THEN
21820          DISP "Establish all species with same probable descendancy";
21830          INPUT " pattern? 0=No 1=yes ",Nsft
21840        ELSE
21850          LET Nsft=1
21860        END IF
21870        LET Nsft=(Nsft>0)
21880        IF Nsft THEN
21890          IF Mski THEN
21900            DISP "What is fractional chance of parents descending";
21910            DISP " other species? (default=";VAL$(Prpt);
21920            INPUT ")",Prpt
```

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```
21930              IF Prpt<0 OR Prpt>1 THEN Prpt=FRACT(Prpt)
21940            END IF                      ! endif, Mski else Prpt defaults
21950          IF Gpcs=1 THEN
21960            LET Ruls(1,1)=1
21970          ELSE
21980            FOR Gski=1 TO Gpcs
21990              FOR Sski=1 TO Gpcs
22000                IF Sski=Gski THEN
22010                  LET Ruls(Gski,Sski)=1-Prpt
22020                ELSE
22030                  LET Ruls(Gski,Sski)=Prpt/(Gpcs-1)
22040                END IF
22050              NEXT Sski
22060            NEXT Gski
22070          END IF
22080        END IF                          ! endif, Nsft test
22090        IF NOT Nsft THEN
22100          FOR Gski=1 TO Gpcs             ! up to 9 species
22110            LET Vski=0
22120            LET Ruls(Gski,0)=0
22130            FOR Sski=1 TO Gpcs           ! up to 9 species evolutions
22140              LET Ruls(Gski,Sski)=1/Gpcs! default
22150              IF Mski THEN
22160                DISP "Occupation most probable";
22170                DISP " for species [";VAL$(Sski);
22180                DISP "] descending from parent species [";VAL$(Gski);
22190                INPUT "]?",Ruls(Gski,Sski)
22200              ELSE
22210                IF Gski=Sski THEN
22220                  LET Ruls(Gski,Sski)=1-Prpt
22230                ELSE
22240                  LET Ruls(Gski,Sski)=Prpt/(1-Prpt)
22250                END IF
22260              END IF
22270              LET Vski=Vski+Ruls(Gski,Sski)
22280            NEXT Sski
22290            IF Vski<>0 THEN Vski=1/Vski
22300            IF Vski<>0 THEN              ! normalize evolution requests
22310              FOR Sski=1 TO Gski
22320                LET Ruls(Gski,Sski)=Ruls(Gski,Sski)*Vski
22330              NEXT Sski
22340            END IF
22350          NEXT Gski
22360        END IF                           ! endif, not Nsft test
22370      END IF                             ! endif, Rset test
22380    END IF                               ! endif, Shv=0 test
22390    IF Mski THEN                         ! imprint?
22400      DISP "Use which species as the STARTER evolutionary pattern?";
22410      DISP " (O=from user, default=";VAL$(Vlv);
22420      INPUT ")",Vlv
22430      LET Relay(4)=Vlv
22440    END IF
22450    IF Shv=0 THEN
22460      FOR Sski=0 TO Qski               ! set up of 2x2x2 Pixel fill
22470        LET Xski=BIT(Sski,0)+BIT(Sski,1)*Mlk1+BIT(Sski,2)*Mlk2+1
```

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```
22480          IF Vlv=0 THEN
22490            LET Pixl(Xski)=BIT(BIT(Sski,0)+BIT(Sski,1)+BIT(Sski,2),0)+1
22500            DISP "Give STARTER species at Pixel(";VAL$(BIT(Sski,0)+1);
22510            IF Qski>1 THEN DISP ",";VAL$(BIT(Sski,1)+1);
22520            IF Qski>3 THEN DISP ",";VAL$(BIT(Sski,2)+1);
22530            INPUT ")",Pixl(Xski)
22540          ELSE
22550            LET Pixl(Xski)=Ruls(Vlv,Sski)
22560          END IF
22570       NEXT Sski
22580     ELSE                                ! initial random fill Shv<>0
22590       IF Rset THEN                      ! fill pixels directly fr Ruls
22600         LET Mdl=0
22610         LET Kski=0
22620         FOR Sski=Clmx TO 1 STEP -1
22630           WHILE Mdl<1 AND Kski<=Gpcs
22640             LET Kski=Kski+1            ! current species fill
22650             IF Mski THEN
22660               DISP "How many STARTER pixels for species [";VAL$(Kski);
22670               DISP "] (up to ";VAL$(Sski);
22680               INPUT ")",Mdl
22690             ELSE
22700               IF Kski=Gski THEN
22710                 LET Mdl=(1-Prpt)*Qski+.5
22720               ELSE
22730                 LET Mdl=Prpt*Qski
22740               END IF
22750             END IF                    ! endif, Mski=0 test
22760           END WHILE                   ! endif, Mdl<1 test
22770           LET Pixl(Sski)=Kski
22780           LET Mdl=Mdl-1
22790         NEXT Sski
22800       ELSE                            ! else Rset=0, get volume fractions
22810         IF Mski THEN
22820           LET Vski=0
22830           FOR Sski=1 TO Gpcs
22840             IF Vlv=0 THEN DISP "STARTER/";
22850             DISP "CONVERGENCE occupation value";
22860             DISP " saught for species [";VAL$(Sski);
22870             INPUT "]",Dmd(Sski)
22880             LET Vski=Vski+Dmd(Sski)
22890           NEXT Sski
22900           IF Vski=0 THEN
22910             LET Vski=1/Gpcs
22920           ELSE
22930             LET Vski=1/Vski
22940           END IF
22950           FOR Sski=1 TO Gpcs          ! normalize volume fractions
22960             LET Dmd(Sski)=Dmd(Sski)*Vski
22970           NEXT Sski
22980         END IF                        ! endif, else use default Dmd
22990         LET Dv=SUM(Dmd)
23000         IF Dv=0 THEN                   ! if 0,form default demands
23010           FOR Sski=1 TO Gpcs
23020             IF Vlv=0 OR Gpcs=1 THEN
```

```
23030                 LET Dmd(Sski)=1/Gpcs      ! flat Demands
23040              ELSE
23050                IF Sski=Vlv THEN
23060                  LET Dmd(Sski)=1-Prpt    ! proportionate Demands
23070                ELSE
23080                  LET Dmd(Sski)=Prpt/(Gpcs-1)
23090                END IF
23100              END IF
23110           NEXT Sski
23120         END IF
23130         LET Vski=0
23140         LET Kski=0
23150         FOR Sski=1 TO Gpcs            !  fill pixels according to demands
23160           IF Vlv=0 THEN
23170             LET Vski=Vski+Dmd(Sski)*Clmx
23180           ELSE
23190             LET Vski=Vski+Ruls(Vlv,Sski)*Clmx
23200           END IF
23210           WHILE Kski<INT(Vski+.5)
23220             LET Kski=Kski+1
23230             LET Pixl(Kski)=Sski
23240           END WHILE
23250         NEXT Sski
23260       END IF                          ! endif, getting vol fractions
23270       FOR Sski=1 TO SHIFT(Clmx,1)
23280         REPEAT                         ! uses 1st 2 bit triples=6 bits total
23290           LET Nsft=INT(RND*64)
23300         UNTIL Nsft<64                  ! & mask out what is needed
23310         LET Mdl=BINAND(SHIFT(Nsft,3),Qski)+1
23320         LET Nsft=BINAND(Nsft,Qski)+1
23330         LET Kski=Pixl(Mdl)
23340         LET Pixl(Mdl)=Pixl(Nsft)
23350         LET Pixl(Nsft)=Kski
23360       NEXT Sski
23370       FOR Sski=Qski TO 0 STEP -1        ! move Pixels outward
23380         LET Xski=BIT(Sski,0)+BIT(Sski,1)*Mlk1+BIT(Sski,2)*Mlk2+1
23390         LET Pixl(Xski)=Pixl(Sski+1)
23400         IF Xski<>Sski+1 THEN LET Pixl(Sski+1)=0
23410       NEXT Sski
23420     END IF                             ! endif, Shv=0 test, imprinting
23430     IF Rset 1 THEN                     ! form numbering sequence
23440       FOR Sski=0 TO Qski               ! to be shuffled later
23450         LET Ncs(Sski)=Sski
23460       NEXT Sski
23470     END IF
23480     LET Dv=0                           ! Total servo volume request
23490     IF Shv<>0 AND NOT Rset THEN
23500       LET Dv=SUM(Dmd)
23510       IF Dv<>1 THEN PRINT " Norm? SERVO vol =";Dv;"in SUB evolv"
23520     END IF
23530     FOR Gski=1 TO Gens
23540       IF Dv>0 THEN
23550         MAT Pcs=(0)
23560         LET Kski=0
23570         FOR Sski=1 TO Cnk              ! tally for adjusting
```

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```
23580            LET Pcs(Pixl(Sski))=Pcs(Pixl(Sski))+1
23590            IF Pixl(Sski)>0 THEN Kski=Kski+1
23600         NEXT Sski
23610         FOR Sski=1 TO Gpcs
23620            IF Kski=0 THEN
23630               LET Ruls(0,Sski)=0
23640            ELSE
23650               LET Ruls(0,Sski)=0            ! estimate probable fills
23660               FOR Xski=1 TO Gpcs
23670                  LET Ruls(0,Sski)=Ruls(0,Sski)+(Pcs(Xski)/Kski)*Ruls(Xski,Sski)
23680               NEXT Xski                     ! servo coefficients
23690               LET Ruls(0,Sski)=(Dmd(Sski)-Ruls(0,Sski))
23700            END IF
23710         NEXT Sski
23720      END IF
23730      FOR Zski=BINAND(-2,Zmax+1)-1 TO 1 STEP -2 ! 2 fold
23740        FOR Yski=BINAND(-2,Ymax+1)-1 TO 1 STEP -2
23750          FOR Xski=BINAND(-2,Xmax+1)-1 TO 1 STEP -2
23760             LET Fadr=Xski+(Yski-1)*Xmax+(Zski-1)*Mlk2 ! new address
23770             LET Sadr=SHIFT(Xski+1,1)+SHIFT(Yski-1,1)*Xmax
23780             LET Sadr=Sadr+SHIFT(Zski-1,1)*Mlk2 ! source address
23790             LET Rlr=Pixl(Sadr)          ! Pixel to be 2 folded
23800             LET Pixl(Sadr)=0
23810             IF Shv<>0 AND Rset=1 THEN ! shuffle the sequencing
23820               FOR Sski=1 TO SHIFT(Clmx,1)
23830                 REPEAT                 ! uses 1st 2 bit triples=6 bits total
23840                   LET Nsft=INT(RND*64)
23850                 UNTIL Nsft<64          ! & mask out what is needed
23860                 LET Mdl=BINAND(SHIFT(Nsft,3),Qski)
23870                 LET Nsft=BINAND(Nsft,Qski)
23880                 LET Kski=Ncs(Mdl)
23890                 LET Ncs(Mdl)=Ncs(Nsft)
23900                 LET Ncs(Nsft)=Kski
23910               NEXT Sski
23920             END IF
23930             FOR Sski=0 TO Qski
23940               LET Kski=BIT(Sski,0)+BIT(Sski,1)*Mlk1+BIT(Sski,2)*Mlk2
23950               LET Kski=Kski+Fadr       ! Final new address
23960               IF Rlr=0 OR Rlr>Gpcs THEN
23970                 LET Pixl(Kski)=0
23980               ELSE
23990                 IF Shv=0 OR Rset THEN ! Fill by numbers in Ruls
24000                   LET Pixl(Kski)=Ruls(Rlr,Ncs(Sski))
24010                 ELSE                  ! Fill by probabilities
24020                   LET Agen=RND
24030                   LET Vski=0
24040                   LET Mdl=0
24050                   REPEAT
24060                     LET Mdl=Mdl+1
24070                     LET Vski=Vski+Ruls(Rlr,Mdl)+Ruls(0,Mdl)
24080                   UNTIL Vski>=Agen OR Mdl=Gpcs
24090                   LET Pixl(Kski)=Mdl
24100                 END IF
24110               END IF
24120             NEXT Sski
```

```
24130          NEXT Xski
24140          NEXT Yski
24150        NEXT Zski
24160      NEXT Gski
24170      LET Kski=0
24180      FOR Sski=1 TO Cnk
24190        LET Kski=Kski+(Pixl(Sski)=0)
24200      NEXT Sski
24210      IF Kski>0 THEN PRINT Kski;"empty? pixels returned, SUB evolv"
24220      DEALLOCATE Ruls(*)                    ! Bye-bye variable sub arrays
24230 SUBEND
```
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