Electromagnetic wave propagation in complex dispersive media

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Workshop on Quantification of Uncertainties in Material Science
January 15, 2016
A Polynomial Chaos Method for Microscale Modeling

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2. Maxwell-Debye
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Acknowledgments

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A general (phenomenological) material model that arises from considerations of the multi-scale nature of the spatial microstructure of a broad class of materials (e.g., glassy, soils, biological tissues, and amorphous polymers). \(^a\)


Corresponds to a fractional psuedo-differential equation model in the time domain, not suitable for efficient simulation.
Maxwell’s Equations

\[ \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}, \text{ in } (0, T) \times D \]  
(Faraday)

\[ \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} - \nabla \times \mathbf{H} = \mathbf{0}, \text{ in } (0, T) \times D \]  
(Ampere)

\[ \nabla \cdot \mathbf{D} = \nabla \cdot \mathbf{B} = 0, \text{ in } (0, T) \times D \]  
(Poisson/Gauss)

\[ \mathbf{E}(0, x) = \mathbf{E}_0; \mathbf{H}(0, x) = \mathbf{H}_0, \text{ in } D \]  
(Initial)

\[ \mathbf{E} \times \mathbf{n} = \mathbf{0}, \text{ on } (0, T) \times \partial D \]  
(Boundary)

\begin{align*}
\mathbf{E} &= \text{Electric field vector} \\
\mathbf{H} &= \text{Magnetic field vector} \\
\mathbf{J} &= \text{Current density} \\
\mathbf{D} &= \text{Electric flux density} \\
\mathbf{B} &= \text{Magnetic flux density} \\
\mathbf{n} &= \text{Unit outward normal to } \partial \Omega
\end{align*}
Maxwell’s equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

\[
\begin{align*}
D &= \varepsilon E + P \\
B &= \mu H + M \\
J &= \sigma E + J_s
\end{align*}
\]

- \(P\) = Polarization
- \(M\) = Magnetization
- \(J_s\) = Source Current
- \(\varepsilon\) = Electric permittivity
- \(\mu\) = Magnetic permeability
- \(\sigma\) = Electric Conductivity

where \(\varepsilon = \varepsilon_0 \varepsilon_\infty\) and \(\mu = \mu_0 \mu_r\).
We can usually define $P$ in terms of a convolution

$$P(t, x) = g \ast E(t, x) = \int_0^t g(t - s, x; q)E(s, x)ds,$$

where $g$ is the dielectric response function (DRF).

In the frequency domain $\hat{D} = \epsilon \hat{E} + \hat{g}\hat{E} = \epsilon_0\epsilon(\omega)\hat{E}$, where $\epsilon(\omega)$ is called the complex permittivity.

$\epsilon(\omega)$ described by the polarization model
Figure: Real part of $\epsilon(\omega)$, $\epsilon$, or the permittivity [GLG96]. Note: up to 10% spread in measurements was observed, but only averages were published.
Figure: Imaginary part of $\epsilon(\omega)/\omega$, $\sigma$, or the conductivity.
Polarization Models

\[ P(t, x) = g \ast E(t, x) = \int_0^t g(t - s, x; q)E(s, x)ds, \]

- Debye model [1929] \( q = [\epsilon_\infty, \epsilon_d, \tau] \)
  
  \[ g(t, x) = \epsilon_0 \epsilon_d / \tau \, e^{-t/\tau} \]
  
  or \( \tau \dot{P} + P = \epsilon_0 \epsilon_d E \)

  or \( \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1 + i\omega \tau} \)

  with \( \epsilon_d := \epsilon_s - \epsilon_\infty \) and \( \tau \) a relaxation time.
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  with \( \epsilon_d := \epsilon_s - \epsilon_\infty \) and \( \tau \) a relaxation time.

- Cole-Cole model [1936] (heuristic generalization)
  \( q = [\epsilon_\infty, \epsilon_d, \tau, \alpha] \)
  
  \[ \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1 + (i\omega \tau)^\alpha} \]
Polarization Models

\[ P(t, x) = g \ast E(t, x) = \int_0^t g(t - s, x; q) E(s, x) \, ds, \]

- Debye model [1929] \( q = [\epsilon_\infty, \epsilon_d, \tau] \)
  \[ \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1 + i\omega\tau} \]

- Cole-Cole model [1941] \( q = [\epsilon_\infty, \epsilon_d, \tau, \alpha] \)
  \[ \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1 + (i\omega\tau)^\alpha} \]

- Havriliak-Negami model [1967] \( q = [\epsilon_\infty, \epsilon_d, \tau, \alpha, \beta] \)
  \[ \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{(1 + (i\omega\tau)^\alpha)^\beta} \]
Distributions of Relaxation Times

The macroscopic Debye polarization model can be derived from microscopic dipole formulations by passing to a limit over the molecular population [see, Elliot1993].
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- Empirical measurements suggest a log-normal or Beta distribution [Bottcher-Bordewijk1978].
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- One can show that the S-N (and Cole-Cole) model corresponds to a continuous distribution “… it is possible to calculate the necessary distribution function by the method of Fuoss and Kirkwood.” [Cole-Cole1941].
- “Continuous spectrum relaxation functions” are also common in viscoelastic models.
Figure: Real part of $\epsilon(\omega)$, $\epsilon$, or the permittivity [REU2008].
Figure: Imaginary part of $\epsilon(\omega)/\omega$, $\sigma$, or the conductivity [REU2008].
To account for the effect of possible multiple parameter sets $\mathbf{q}$, consider the following polydisperse DRF

$$h(t, x; F) = \int_Q g(t, x; \mathbf{q})dF(\mathbf{q}),$$

where $Q$ is some admissible set and $F \in \mathcal{P}(Q)$. Then the polarization becomes:

$$P(t, x; F) = \int_0^t h(t - s, x; F)E(s, x)ds.$$
Random Polarization

Alternatively we can define the random polarization $\mathcal{P}(t, x; \tau)$ to be the solution to

$$\tau \dot{\mathcal{P}} + \mathcal{P} = \epsilon_0 \epsilon_d E$$

where $\tau$ is a random variable with PDF $f(\tau)$, for example,

$$f(\tau) = \frac{1}{\tau_b - \tau_a}$$

for a uniform distribution.
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for a uniform distribution.

The electric field depends on the macroscopic polarization, which we take to be the expected value of the random polarization at each point $(t, x)$

$$\mathbf{P}(t, x; F) = \int_{\tau_a}^{\tau_b} \mathcal{P}(t, x; \tau) f(\tau) d\tau.$$
Polynomial Chaos

Apply Polynomial Chaos (PC) method to approximate each spatial component of the random polarization

\[ \tau \dot{\mathcal{P}} + \mathcal{P} = \epsilon_0 \epsilon_d E, \quad \tau = \tau(\xi) = \tau_r \xi + \tau_m, \quad \xi \sim F \]

resulting in

\[ (\tau_r M + \tau_m I) \dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0 \epsilon_d E \hat{e}_1 \]

or

\[ A \ddot{\vec{\alpha}} + \vec{\alpha} = \vec{f} . \]
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\[ A \dot{\vec{\alpha}} + \vec{\alpha} = \vec{f}. \]

The electric field depends on the macroscopic polarization, the expected value of the random polarization at each point \((t, x)\), which is

\[ P(t, x; F) = \mathbb{E}[\mathcal{P}] \approx \alpha_0(t, x). \]
Maximum Difference Calculated for different values of $p$ and $r$

Maximum Error

- $r = 1.00\tau$
- $r = 0.75\tau$
- $r = 0.50\tau$
- $r = 0.25\tau$

(N.L. Gibson, OSU)
Comparison of simulations to data [Armentrout-G., 2011].
Comparison of initial to final distribution [Armentrout-G., 2011].

(N.L. Gibson, OSU)
Distributions, noise = 0.1, refinement = 1, test = 5

Initial J = 9.59699
Optimal J = 3.02332
Actual J = 3.02348

(N.L. Gibson, OSU)
In a polydispersive Debye material, we have

\[ \mu_0 \frac{\partial H}{\partial t} = -\nabla \times E, \quad (1a) \]

\[ \epsilon_0 \epsilon_\infty \frac{\partial E}{\partial t} = \nabla \times H - \frac{\partial P}{\partial t} - J \quad (1b) \]

\[ \tau \frac{\partial P}{\partial t} + P = \epsilon_0 \epsilon_d E \quad (1c) \]

with

\[ P(t, x; F) = \int_{\tau_a}^{\tau_b} P(t, x; \tau) dF(\tau). \]
The dispersion relation for the system (1) is given by

\[ \frac{\omega^2}{c^2} \epsilon(\omega) = \| k \|^2 \]

where the expected complex permittivity is given by

\[ \epsilon(\omega) = \epsilon_\infty + \epsilon_d E \left[ \frac{1}{1 + i\omega \tau} \right] . \]

Where \( k \) is the wave vector and \( c = 1/\sqrt{\mu_0 \epsilon_0} \) is the speed of light.
**Theorem (G., 2015)**

The dispersion relation for the system (1) is given by

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Where \( k \) is the wave vector and \( c = 1/\sqrt{\mu_0 \varepsilon_0} \) is the speed of light.

Note: for a uniform distribution on \([\tau_a, \tau_b]\), this has an analytic form since

\[ \mathbb{E} \left[ \frac{1}{1 + i\omega \tau} \right] = \frac{1}{\omega(\tau_b - \tau_a)} \left[ \arctan(\omega \tau) + i \frac{1}{2} \ln \left(1 + (\omega \tau)^2\right) \right]_{\tau = \tau_a}^{\tau = \tau_b}. \]

The exact dispersion relation can be compared with a discrete dispersion relation to determine the amount of dispersion error.
Finite Difference Time Domain (FDTD)

We now choose a discretization of the Maxwell-PC Debye model. Note that any scheme can be used independent of the spectral approach in random space employed here.

The Yee Scheme (FDTD)

- This gives an explicit second order accurate scheme in time and space.
- It is conditionally stable with the CFL condition

\[
\nu := \frac{c\Delta t}{h} \leq \frac{1}{\sqrt{d}}
\]

where \( \nu \) is called the Courant number and \( c_\infty = 1/\sqrt{\mu_0\varepsilon_0\varepsilon_\infty} \) is the fastest wave speed and \( d \) is the spatial dimension, and \( h \) is the (uniform) spatial step.
- The Yee scheme can exhibit numerical dispersion and dissipation.
Yee Scheme for Maxwell-Debye System (in 1D)

\[ \mu_0 \frac{\partial H}{\partial t} = -\frac{\partial E}{\partial z} \]
\[ \epsilon_0 \epsilon_\infty \frac{\partial E}{\partial t} = -\frac{\partial H}{\partial z} - \frac{\partial P}{\partial t} \]
\[ \tau \frac{\partial P}{\partial t} = \epsilon_0 \epsilon_d E - P \]

become

\[ \mu_0 \frac{H_{j+\frac{1}{2}}^{n+1} - H_{j+\frac{1}{2}}^n}{\Delta t} = -\frac{E_{j+\frac{1}{2}}^{n+\frac{1}{2}} - E_{j}^{n+\frac{1}{2}}}{\Delta z} \]
\[ \epsilon_0 \epsilon_\infty \frac{E_{j}^{n+\frac{1}{2}} - E_{j}^{n-\frac{1}{2}}}{\Delta t} = -\frac{H_{j+\frac{1}{2}}^n - H_{j-\frac{1}{2}}^n}{\Delta z} - \frac{P_{j}^{n+\frac{1}{2}} - P_{j}^{n-\frac{1}{2}}}{\Delta t} \]
\[ \tau \frac{P_{j}^{n+\frac{1}{2}} - P_{j}^{n-\frac{1}{2}}}{\Delta t} = \epsilon_0 \epsilon_d \frac{E_{j}^{n+\frac{1}{2}} + E_{j}^{n-\frac{1}{2}}}{2} - \frac{P_{j}^{n+\frac{1}{2}} + P_{j}^{n-\frac{1}{2}}}{2} . \]
(Petropolous1994) showed that for the Yee scheme applied to the Maxwell-Debye, the discrete dispersion relation can be written

\[ \frac{\omega^2}{c^2} \epsilon_\Delta(\omega) = K_\Delta^2 \]

where the discrete complex permittivity is given by

\[ \epsilon_\Delta(\omega) = \epsilon_\infty + \epsilon_d \left( \frac{1}{1 + i\omega_\Delta \tau_\Delta} \right) \]

with discrete (mis-)representations of \( \omega \) and \( \tau \) given by

\[ \omega_\Delta = \sin \left( \frac{\omega \Delta t}{2} \right) \Delta t / 2, \quad \tau_\Delta = \sec(\omega \Delta t / 2) \tau. \]
The quantity $K_\Delta$ is given by

$$K_\Delta = \frac{\sin (k\Delta z/2)}{\Delta z/2}$$

in 1D and is related to the symbol of the discrete first order spatial difference operator by

$$iK_\Delta = \mathcal{F}(\mathcal{D}_{1,\Delta z}).$$

In this way, we see that the left hand side of the discrete dispersion relation

$$\frac{\omega^2}{c^2} \epsilon_\Delta(\omega) = K^2_\Delta$$

is unchanged when one moves to higher order spatial derivative approximations [Bokil-G,2012] or even higher spatial dimension [Bokil-G,2013].
Theorem (G., 2015)

The discrete dispersion relation for the Maxwell-PC Debye FDTD scheme is given by

\[
\frac{\omega^2}{c^2} \epsilon_\Delta(\omega) = K_\Delta^2
\]

where the discrete expected complex permittivity is given by

\[
\epsilon_\Delta(\omega) := \epsilon_\infty + \epsilon_d \hat{e}_1^T \left( I + i\omega A_\Delta \right)^{-1} \hat{e}_1
\]

and the discrete PC matrix is given by

\[
A_\Delta := \sec(\omega \Delta t/2) A.
\]

The definitions of the parameters \( \omega_\Delta \) and \( K_\Delta \) are the same as before. Recall the exact complex permittivity is given by

\[
\epsilon(\omega) = \epsilon_\infty + \epsilon_d \text{Re} \left[ \frac{1}{1 + i\omega \tau} \right].
\]
Dispersion Error

We define the phase error $\Phi$ for a scheme applied to a model to be

$$
\Phi = \left| \frac{k_{EX} - k_{\Delta}}{k_{EX}} \right|,
$$

(2)

where the numerical wave number $k_{\Delta}$ is implicitly determined by the corresponding dispersion relation and $k_{EX}$ is the exact wave number for the given model.
Dispersion Error

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where the numerical wave number $k_{\Delta}$ is implicitly determined by the corresponding dispersion relation and $k_{EX}$ is the exact wave number for the given model.

- We wish to examine the phase error as a function of $\omega \Delta t$ in the range $[0, \pi]$. $\Delta t$ is determined by $h_\tau \tau_m$, while $\Delta x = \Delta y$ determined by CFL condition.
- We note that $\omega \Delta t = 2\pi / N_{ppp}$, where $N_{ppp}$ is the number of points per period, and is related to the number of points per wavelength as, $N_{ppw} = \sqrt{\epsilon_\infty \nu} N_{ppp}$.
- We assume a uniform distribution and the following parameters which are appropriate constants for modeling aqueous Debye type materials:

$$\epsilon_\infty = 1, \quad \epsilon_s = 78.2, \quad \tau_m = 8.1 \times 10^{-12} \text{ sec}, \quad \tau_r = 0.5 \tau_m.$$
**Figure**: Plots of phase error at $\theta = 0$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$. 
**Figure**: Plots of phase error at $\theta = 0$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.001$. 
Figure: Log plots of phase error versus $\theta$ with fixed $\omega = 1/\tau_m$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.01$. Legend indicates degree $M$ of the PC expansion.
Figure: Log plots of phase error versus $\theta$ with fixed $\omega = 1/\tau_m$ for (left column) $\tau_r = 0.5\tau_m$, (right column) $\tau_r = 0.9\tau_m$, using $h_\tau = 0.001$. Legend indicates degree $M$ of the PC expansion.
Conclusions

- We have presented a random ODE model for polydispersive Debye media

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\textsuperscript{1}GIBSON, N. L., A Polynomial Chaos Method for Dispersive Electromagnetics, \textit{Comm. in Comp. Phys.}, 2015
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Conclusions

- We have presented a random ODE model for polydispersive Debye media.
- We described an efficient numerical method utilizing polynomial chaos (PC) and finite difference time domain (FDTD).
- Exponential convergence in the number of PC terms was demonstrated.
- We have proven (conditional) stability of the scheme via energy decay (not shown).
- We have derived a discrete dispersion relation and computed phase errors.

Polynomial Chaos: Simple example

Consider the first order, constant coefficient, linear IVP

\[ \dot{y} + ky = g, \quad y(0) = y_0 \]

with

\[ k = k(\xi) = \xi, \quad \xi \sim \mathcal{N}(0, 1), \quad g(t) = 0. \]

We can represent the solution \( y \) as a Polynomial Chaos (PC) expansion in terms of (normalized) orthogonal Hermite polynomials \( H_j \):

\[ y(t, \xi) = \sum_{j=0}^{\infty} \alpha_j(t) \phi_j(\xi), \quad \phi_j(\xi) = H_j(\xi). \]

Substituting into the ODE we get

\[ \sum_{j=0}^{\infty} \dot{\alpha}_j(t) \phi_j(\xi) + \sum_{j=0}^{\infty} \alpha_j(t) \xi \phi_j(\xi) = 0. \]
Appendix

Polynomial Chaos

Triple recursion formula

\[ \sum_{j=0}^{\infty} \dot{\alpha}_j(t) \phi_j(\xi) + \sum_{j=0}^{\infty} \alpha_j(t) \xi \phi_j(\xi) = 0. \]

We can eliminate the explicit dependence on \( \xi \) by using the triple recursion formula for Hermite polynomials

\[ \xi H_j = jH_{j-1} + H_{j+1}. \]

Thus

\[ \sum_{j=0}^{\infty} \dot{\alpha}_j(t) \phi_j(\xi) + \sum_{j=0}^{\infty} \alpha_j(t)(j \phi_{j-1}(\xi) + \phi_{j+1}(\xi)) = 0. \]
In order to approximate $y$ we wish to find a finite system for at least the first few $\alpha_i$.

We take the weighted inner product with the $i$th basis, $i = 0, \ldots, p$,

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t) \langle \phi_j, \phi_i \rangle_W + \alpha_j(t) (j \langle \phi_{j-1}, \phi_i \rangle_W + \langle \phi_{j+1}, \phi_i \rangle_W) = 0,$$

where

$$\langle f(\xi), g(\xi) \rangle_W := \int f(\xi) g(\xi) W(\xi) d\xi.$$
Galerkin Projection onto \( \text{span}(\{\phi_i\}_{i=0}^p) \)

In order to approximate \( y \) we wish to find a finite system for at least the first few \( \alpha_i \).
We take the weighted inner product with the \( i \)th basis, \( i = 0, \ldots, p \),

\[
\sum_{j=0}^{\infty} \dot{\alpha}_j(t) \langle \phi_j, \phi_i \rangle_W + \alpha_j(t)(j \langle \phi_{j-1}, \phi_i \rangle_W + \langle \phi_{j+1}, \phi_i \rangle_W) = 0,
\]

where

\[
\langle f(\xi), g(\xi) \rangle_W := \int f(\xi)g(\xi)W(\xi)d\xi.
\]

By orthogonality, \( \langle \phi_j, \phi_i \rangle_W = \langle \phi_i, \phi_i \rangle_W \delta_{ij} \), we have

\[
\dot{\alpha}_i \langle \phi_i, \phi_i \rangle_W + (i + 1)\alpha_{i+1} \langle \phi_i, \phi_i \rangle_W + \alpha_{i-1} \langle \phi_i, \phi_i \rangle_W = 0, \quad i = 0, \ldots, p.
\]
Deterministic ODE system

Let $\vec{\alpha}$ represent the vector containing $\alpha_0(t), \ldots, \alpha_p(t)$. Assuming $\alpha_{-1}(t), \alpha_{p+1}(t)$, etc., are identically zero, the system of ODEs can be written

$$\dot{\vec{\alpha}} + M\vec{\alpha} = \vec{0},$$

with

$$M = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & p \\ & & & 1 & 0 \end{bmatrix}$$

The degree $p$ PC approximation is $y(t, \xi) \approx y^p(t, \xi) = \sum_{j=0}^{p} \alpha_j(t) \phi_j(\xi)$. The mean value $E[y(t, \xi)] \approx E[y^p(t, \xi)] = \alpha_0(t)$. The variance $Var(y(t, \xi)) \approx \sum_{j=1}^{p} \alpha_j(t)^2$. 
Figure: Convergence of error with Gaussian random variable by Hermitian-chaos.
Generalizations

Consider the non-homogeneous IVP

\[ \dot{y} + ky = g(t), \quad y(0) = y_0 \]

with

\[ k = k(\xi) = \sigma \xi + \mu, \quad \xi \sim \mathcal{N}(0, 1), \]

then

\[ \dot{\alpha}_i + \sigma [(i + 1)\alpha_{i+1} + \alpha_{i-1}] + \mu \alpha_i = g(t)\delta_{0i}, \quad i = 0, \ldots, p, \]

or the deterministic ODE system is

\[ \dot{\alpha} + (\sigma M + \mu I)\alpha = g(t)e_1. \]

Note that the initial condition for the PC system is \( \alpha(0) = y_0 e_1. \)
Generalizations

For any choice of family of orthogonal polynomials, there exists a triple recursion formula. Given the arbitrary relation

\[ \xi \phi_j = a_j \phi_{j-1} + b_j \phi_j + c_j \phi_{j+1} \]

(with \( \phi_{-1} = 0 \)) then the matrix above becomes

\[
M = \begin{bmatrix}
  b_0 & a_1 & & \\
  c_0 & b_1 & a_2 & \\
  & \ddots & \ddots & \ddots \\
  & & \ddots & \ddots & a_p \\
  & & & c_{p-1} & b_p
\end{bmatrix}
\]
Generalized Polynomial Chaos

Table: Popular distributions and corresponding orthogonal polynomials.

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Polynomial</th>
<th>Support</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian</td>
<td>Hermite</td>
<td>$(-\infty, \infty)$</td>
</tr>
<tr>
<td>gamma</td>
<td>Laguerre</td>
<td>$[0, \infty)$</td>
</tr>
<tr>
<td>beta</td>
<td>Jacobi</td>
<td>$[a, b]$</td>
</tr>
<tr>
<td>uniform</td>
<td>Legendre</td>
<td>$[a, b]$</td>
</tr>
</tbody>
</table>

Note: lognormal random variables may be handled as a non-linear function (e.g., Taylor expansion) of a normal random variable.