Peridynamics for coupled field equations

E. Madenci, S. Oterkus
The University of Arizona
• Fully Coupled Thermomechanics
• Hygrothermomechanics
• Fully Coupled Fluid Flow and Deformation Field
• Electromigration
Peridynamic Equation of Motion

Equation of motion of a material point at $x$ (CCM)

$$\rho(x)\ddot{u}(x,t) = \nabla \cdot \sigma + b(x,t)$$

Equation of motion of a material point at $x$ (PD)

$$\rho(x)\ddot{u}(x,t) = \int_{H} \left( t(u' - u, x' - x, t) - t'(u' - u, x' - x, t) \right) dH + b(x,t)$$

Peridynamic Equation of Motion

Ordinary state-based

\[ \rho(x) \ddot{u}(x, t) = \int_{H} \left( \dot{t}(u' - u, x' - x, t) - \dot{t}'(u' - u, x' - x, t) \right) dH + b(x, t) \]

Bond-based \( t' = -t \) \( \Rightarrow \)

\[ \rho(x) \ddot{u}(x, t) = \int_{H} \left( f(u' - u, x' - x, t) \right) dH + b(x, t) \]
Failure in Peridynamics

\[ \rho \ddot{u}(x_k, t) = \sum_{j=1}^{N} \mu(t(u_j, u_k, x_j, x_k, t) - t'\left(u_j, u_k, x_j, x_k, t\right))V_j + b(x_k, t) \]

\[ \mu(t, \xi) = \begin{cases} 
1 & \text{if } s(t', \xi) < s_0 \text{ for all } 0 \leq t' \leq t \\
0 & \text{otherwise} \end{cases} \]

**Elasticity-CCM**

**Stress:** \( T_i = \sigma_{ji} n_j \)

**Equations of motion:**
\[
\rho \ddot{u}_i(x,t) = \sigma_{ij,j} + b_i(x,t)
\]

**Balance of angular momentum:**
\( \sigma_{ij} = \sigma_{ji} \)

**Constitutive relations:**
\[
\sigma_{ij} = \frac{\partial W}{\partial \varepsilon_{ij}}
\]
\[
W = \frac{1}{2} K(\varepsilon_{\ell\ell})^2 + 2\mu \left( \frac{1}{2} \varepsilon_{ij} \varepsilon_{ij} - \frac{1}{6} (\varepsilon_{\ell\ell})^2 \right)
\]
\[
= \frac{1}{2} K(\theta)^2 + \frac{1}{2\mu} J^2
\]
\[
\theta = \varepsilon_{\ell\ell}
\]
\[
\varepsilon_{ij} = \frac{1}{2\mu} \sigma_{ij} - \frac{1}{2\mu} \frac{1}{(3\lambda + 2\mu)} \sigma_{\ell\ell}\delta_{ij}
\]

**Elasticity-PD**

**Force density vector:** \( t \)

**Equations of motion:**
\[
\rho \ddot{u} = \int_H \left[ t(u' - u, x' - x, t) - t'(u - u', x - x', t) \right] dH + b
\]

**Balance of angular momentum:**
\( t / / (y' - y) \)

**Constitutive relations:**
\[
t = \frac{\partial W}{\partial (|y' - y| |y' - y|)} y' - y
\]
\[
W(x) = a_w \theta^2(x)
\]
\[
\theta(x) = d \int_H \delta s \left( \frac{y' - y \cdot x' - x}{|y' - y| |x' - x|} \right) dH
\]
\[
s = (|y' - y| - |x' - x|)/|x - x|
\]
Diffusion Equations

**Classical**

\[ m_1 \dot{\psi} = m_2 \nabla^2 \psi + s \]

**Peridynamics**

\[ m_1 \dot{\psi}(x, t) = \int_H f(\psi', \psi, x', x, t) dV_{x'} + s(x, t) \]

Exchange of energy/mass between the material points

**Bond constant**

\[ \kappa = \begin{cases} 
\frac{2m_2}{A\delta^2} & (1-D) \\
\frac{6m_2}{\pi h\delta^3} & (2-D) \\
\frac{6m_2}{\pi \delta^4} & (3-D) 
\end{cases} \]

**Flux**

\[ q = -m_2 \nabla \psi' \]

\[ q = -\frac{1}{2} \int_H \kappa [\psi'(x', t) - \psi(x, t)] \frac{(x' - x)}{|x' - x|} dV_{x'} \]
Fully Coupled Thermomechanics

Thermal diffusion with structural heating term:

\[ \rho c_v \dot{T} = k_T T_{,ii} - \beta_{cl} \Theta_o \dot{u}_{j,j} \]

Classical

Equation of motion with thermal load term:

\[ \rho \frac{\partial^2 u}{\partial t^2} = \nabla \sigma + b + \beta_{cl} T_{,i} \]

Peridynamics

Thermal diffusion with structural heating term:

\[ \rho c_v \dot{T}(x,t) = \int_H \left( \kappa_T \frac{T'(x',t) - T(x,t)}{|x' - x|} \right) dV \]

\[ -\int_H \left( \Theta_o \frac{c}{2} \alpha \dot{\varepsilon} \right) dV + q_T(x,t) \]

Peridynamics

Equation of motion with thermal load term:

\[ \rho \ddot{u}(x,t) = \int_H c \left( s - \alpha T \right) \frac{y' - y}{|y' - y|} dV + b(x,t) \]
Hygrothermomechanics

Thermal diffusion equation

\[ \rho c_v \frac{dT}{dt}(x,t) = \int_H \left( \kappa_T \frac{T'(x',t) - T(x,t)}{|x' - x|} \right) dV' \]

Moisture diffusion equation

\[ \frac{dC}{dt}(x,t) = \int_H \kappa_M \frac{C'(x',t) - C(x,t)}{|x' - x|} dV_x' \]

Equation of motion

\[ \rho \ddot{u}(x,t) = \int_H \left( c \left( s - \alpha \bar{T} \right) + \beta \bar{C}_M + \gamma P_{vapor} \right) \frac{(x' + u') - (x + u)}{|(x' + u') - (x + u)|} dV' + b(x,t) \]

thermal - moisture - vapor pressure
PD Coupled deformation and flow equations

**Classical**

*Flow Equation with mechanical effect*

\[
\frac{1}{Q} \frac{\partial P_f}{\partial t} = \frac{k}{\mu} \nabla^2 P_f - \alpha_B \frac{\partial \varepsilon_{ii}}{\partial t} + \frac{q_f}{\rho}
\]

*Equation of motion with fluid pressure*

\[
\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \sigma + \mathbf{b} - \alpha_B \nabla P
\]

**Peridynamics**

*Mechanical term*

\[
\frac{\dot{P}(\mathbf{x}, t)}{Q_B} = \int_{H} \left( \kappa_P \frac{P(\mathbf{x}', t) - P(\mathbf{x}, t)}{|\mathbf{x}' - \mathbf{x}|} \right) dV - \int_{H} \left( \frac{c}{2} \alpha_B \gamma \dot{\varepsilon} \right) dV + \frac{q_f}{\rho_f}
\]

*Fluid pressure term*

\[
\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{H} c \left( s - \alpha_B \gamma \bar{P} \right) \frac{y' - y}{|y' - y|} dV + \mathbf{b}(\mathbf{x}, t)
\]
Electromigration

Electrical Potential → Temperature Field → Displacement Field

Diffusion of Atoms (or vacancy)

Failure

Change in Structure (void formation)
Thermoelectrical simulation

\[ c_E \dot{\Phi}(x, t) = \int_H \kappa_E \frac{\Phi(x', t) - \Phi(x, t)}{|x' - x|} dV_{x'} \]

\[ j(x, t) = -\frac{1}{2} \int_H f_E (\Phi', \Phi, x', x, t)(x' - x) dV_{x'} \]

\[ q_E(x, t) = \frac{1}{k_E} j(x, t) \cdot j(x, t) \]

\[ \rho c_v \dot{T}(x, t) = \int_H f_T (T', T, x', x, t) dV_{x'} + q_E(x, t) \]

Thermomechanical simulation

\[ \rho(x) \ddot{u}(x, t) = \int_H c(s - \alpha T) \frac{v' - v}{|v' - v|} dH + b(x, t) \]

\[ \rho c_v \dot{\Theta}(x, t) = \int_H \kappa_T \frac{\Theta(x', t) - \Theta(x, t)}{|x' - x|} dV' \]
Atomic flux due to electromigration

Classical form

\[ \frac{\partial C_a}{\partial t} + \nabla \cdot (\vec{J}) = 0 \]

\[ \frac{\partial \varepsilon}{\partial t} = -\Omega \nabla \cdot (\vec{J}) \]

\[ \vec{J}_{EM} = \frac{C_a D_a}{kT} Z^* e (\nabla \Phi) \]

PD form

\[ \frac{\partial \varepsilon}{\partial t} = -\frac{\Omega \kappa_f}{2} \int_H \left( J'_x(x', t) - J_x(x, t) \right) \frac{x' - x}{|x' - x|} dV_x \]

\[ \vec{J}_{PD} = \frac{1}{2} \int_H \frac{C_{A,avg} D_{A,avg}}{T_{avg}} \kappa_{EM} \frac{\Phi'(x', t) - \Phi(x, t)}{|x' - x|} (x' - x) dV_{x'} \]
Pressure or Temperature Shock or their combination

$L = 10$
$W = 10$
$H = 1$

Initial conditions
$\bar{T}(\bar{x}, \bar{y}, 0) = 0$
$\bar{u}_x(\bar{x}, \bar{y}, 0) = \bar{u}_y(\bar{x}, \bar{y}, 0) = 0$

Discretization
$N_x = 200$
$N_y = 200$
$\Delta \bar{t} = 0.5 \times 10^{-3}$

Boundary conditions
$\bar{T}_{\bar{x}}(\bar{x} = 10, \bar{y}, \bar{t}) = 0$
$\bar{T}_{\bar{y}}(\bar{x}, \bar{y} = \pm 5, \bar{t}) = 0$
$\bar{u}_x(\bar{x} = 10, \bar{y}, \bar{t}) = \bar{u}_y(\bar{x} = 10, \bar{y}, \bar{t}) = 0$

Pressure Shock
$\bar{T}(\bar{t}) = 0$
$P(\bar{t}) = 0$

Temperature Shock
$P(\bar{t}) = 5\bar{t} \exp(-2\bar{t})$
$\bar{T}(\bar{t}) = 5\bar{t} \exp(-2\bar{t})$

Temperature and Pressure Shock
$P(\bar{t}) = 5\bar{t} \exp(-2\bar{t})$
$\bar{T}(\bar{t}) = 5\bar{t} \exp(-2\bar{t})$
Plate subjected to Pressure Shock

(blue and red - decoupled cases)
(green and purple - coupled cases)

\[ T(t) = 0 \]
\[ P(t) = 5\bar{t} \exp(-2\bar{t}) \]

Plate subjected to Thermal Shock

(blue and red - decoupled cases)

green and purple - coupled cases

\[ P(\bar{t}) = 0 \]
\[ \bar{T}(\bar{t}) = 5\bar{t} \exp(-2\bar{t}) \]

Temperature variations along the centerline in the plate for uncoupled and coupled cases

Displacement variations along the centerline in the plate for uncoupled and coupled cases

Plate under Pressure and Thermal Shock

\[ P(\bar{t}) = 5 \bar{t} \exp(-2\bar{t}) \]
\[ \overline{T}(\bar{t}) = 5\bar{t} \exp(-2\bar{t}) \]

Temperature variations along the centerline in the plate for uncoupled and coupled cases

Displacement variations along the centerline in the plate for uncoupled and coupled cases

Hygrothermomechanics

The electronic package is subjected to absorption for 168h and desorption for 25 min

1-Molding compound
2-Die attach
3-Silicon die
4-Copper

\[ E_1 = 15 \times 10^6 \text{ Pa}, \quad E_2 = 7.4 \times 10^8 \text{ Pa}, \]
\[ E_3 = 163 \times 10^6 \text{ Pa}, \quad E_4 = 129 \times 10^6 \text{ Pa} \]
\[ \beta_1 = 22.2 \times 10^{-5} \text{ m}^3/\text{kg}, \quad \beta_2 = 5.194 \times 10^{-4} \text{ m}^3/\text{kg}, \]
\[ \beta C_{sat1} = 0, \quad \beta C_{sat4} = 0 \]
\[ C_{sat1} = 7.06 \text{ kg/m}^3, C_{sat2} = 6.20 \text{ kg/m}^3, \]
\[ C_{sat3} = 0, \quad C_{sat4} = 0 \]
\[ \alpha_1 = 16 \times 10^{-6} \text{ 1/°K}, \quad \alpha_2 = 52 \times 10^{-6} \text{ 1/°K}, \]
\[ \alpha_3 = 2.6 \times 10^{-6} \text{ 1/°K}, \quad \alpha_4 = 14.3 \times 10^{-6} \text{ 1/°K} \]
\[ \nu_1 = 0.25, \quad \nu_2 = 0.4, \quad \nu_3 = 0.278, \quad \nu_4 = 0.355 \]
\[ \rho_1 = 1180 \text{ kg/m}^3, \quad \rho_2 = 6450 \text{ kg/m}^3, \]
\[ \rho_3 = 2330 \text{ kg/m}^3, \quad \rho_2 = 8940 \text{ kg/m}^3 \]

**During absorption**
\[ D_1 = 2.66 \times 10^{-9} \text{ m}^2/\text{h} \]
\[ D_2 = 45 \times 10^{-9} \text{ m}^2/\text{h} \]

**During desorption**
\[ D_1 = 6.0 \times 10^{-7} \text{ m}^2/\text{h} \]
\[ D_2 = 1.5 \times 10^{-6} \text{ m}^2/\text{h} \]

\[ L_1 = 2.5 \text{ mm}, \quad L_2 = 0.45 \text{ mm}, \quad L_3 = 0.4 \text{ mm}, \quad L_4 = 0.65 \text{ mm} \]
\[ H_1 = 0.2 \text{ mm}, H_2 = 0.05 \text{ mm}, \quad H_3 = 0.4 \text{ mm}, \quad H_4 = 0.35 \text{ mm} \]
\[ h = 0.01 \text{ mm} \]
Wetness distribution after 168h absorption (a) PD (b) ANSYS solution

Wetness distribution after 168h absorption 25 min desorption (a) PD (b) ANSYS solution

Wetness induced vapor pressure distribution (MPa)  Failure prediction
Consolidation

$L = 15 \text{ m}$

$E = 1.0 \times 10^8 \text{ N/m}^2$, $\nu = 1/3$

$Q = 1/1.65 \times 10^{-10} \text{ N/m}^2$

$\kappa = k_p/\mu = 1.02 \times 10^{-9} \text{ m}^4/\text{Ns}$

$\rho = 1900 \text{ kg/m}^3$, $\alpha = 0.5$

**Boundary Conditions**

$P_0 = 1 \times 10^4 \text{ N/m}^2$ \hspace{1cm} $P_f(z = 0, t) = 0$

$u_z(z = L, t) = 0$ \hspace{1cm} $\frac{\partial P_f}{\partial z}(z = L, t) = 0$

**Initial Condition**

$P(z, t = 0) = \nu P_o$

$u_z(z, t = 0) = \alpha_i P_o \left(h - z\right)$

**No normal flow along at the bottom boundary**

Hydraulically pressurized crack

Boundary conditions on the crack surfaces

\[ \sigma_{zz}(z = L/2, x) = -P_o \frac{t}{t_o} \quad L/2 - a < x < L/2 + a \]

\[ P(z = L/2, x) = P_o \frac{t}{t_o} \quad L/2 - a < x < L/2 + a \]

where \( P_o = 2000 \text{Pa}, t = 0.01 \text{s} \)

Boundary conditions on the lateral surfaces

\[ u_x(x = 0, z, t) = 0 \]
\[ u_x(x = W, z, t) = 0 \]
\[ u_z(x, z = 0, t) = 0 \]
\[ u_z(x, z = L, t) = 0 \]
\[ \frac{\partial P}{\partial x}(x = 0, z, t) = 0 \]
\[ \frac{\partial P}{\partial x}(x = W, z, t) = 0 \]
\[ \frac{\partial P}{\partial z}(x, z = 0, t) = 0 \]
\[ \frac{\partial P}{\partial z}(x, z = L, t) = 0 \]

No normal flow along the outer boundaries

Initial Conditions

\[ u_x(x, z, t = 0) = 0, u_z(x, z, t = 0) = 0 \]
\[ \dot{u}_x(x, z, t = 0) = 0, \dot{u}_z(x, z, t = 0) = 0 \]
\[ P(x, z, t = 0) = 0 \]

\[ L = W = 6 \text{m} \]
\[ 2a = 0.3 \text{m} \]
\[ E = 1.0 \times 10^8 \text{N/m}^2, \nu = 1/3 \]
\[ Q = 1/1.65 \times 10^{-10} \text{N/m}^2 \]
\[ \kappa = k_p/\mu = 1.02 \times 10^{-9} \text{m}^4/\text{Ns} \]
\[ \rho = 1900 \text{kg/m}^3, \alpha = 0.1 \]
Hydraulically Pressurized Crack – failure is not allowed

Peridynamic predictions

ANSYS predictions

Fluid pore pressures (Pa)  Vertical Displ. (m)  Horizontal Displ. (m)
Hydraulically Pressurized Crack – failure is allowed

PD solution of fluid pore pressures with crack propagation (Pa)
Electromigration in thin copper wires

Geometric Parameters:

- $L = 100 \mu m$
- $W = W_1 = W_2 = 10 \mu m$
- $L_1 = L_3 = 40 \mu m$
- $L_2 = 10 \mu m$
- $h = 1 \mu m$
- $E = 120 \times 10^8$ N/m$^2$
- $\rho = 8960$ kg/m$^3$
- $k_T = 401$ W/m °K
- $c_v = 385$ J/kg °K
- $k_E = 59.6 \times 10^6$ 1/(m·ohm)
- $Z' = 1.5$
- $m_A = 63.546 \times 10^{-3}$ kg/mol
- $e = 1.602 \times 10^{-19}$ coulomb
- $Q = 3.4877 \times 10^{-23}$ J/vacancy
- $E_v = 1.602 \times 10^{-19}$ J/vacancy
- $D_o = 6.9 \times 10^{-5}$ m$^2$/s
- $\Omega = 1.182 \times 10^{-29}$ m$^3$

Initial conditions:

- $u_x(x, y, t = 0) = 0$
- $u_y(x, y, t = 0) = 0$
- $T(x, y, t = 0) = 0^\circ$ C
- $\Phi(x, y, t = 0) = 0$ volt
- $C_m = 0.01$ vacancies/atom

Boundary conditions:

**Case-1**

- $x = 0$
  - $u_x(x = 0, y, t) = 0$
  - $u_y(x = 0, y, t) = 0$
  - $T(x = 0, y, t) = 0^\circ$ C
  - $\Phi(x = 0, y, t) = -0.12$ volt

- $x = L$
  - $\sigma_{xx}(x = L, y, t) = 0$
  - $\sigma_{yx}(x = L, y, t) = 0$
  - $T(x = L, y) = 0^\circ$ C
  - $\Phi(x = L, y, t) = 0$ volt

- $y = 0$
  - $\sigma_{yy}(x, y = 0, t) = 0$
  - $\sigma_{xy}(x, y = 0, t) = 0$
  - $T(x, y = 0, t) = 0$
  - $\Phi_y(x, y = 0, t) = 0$

- $y = W$
  - $\sigma_{yy}(x, y = W, t) = 0$
  - $\sigma_{xy}(x, y = W, t) = 0$
  - $T(x, y = W, t) = 0$
  - $\Phi_y(x, y = W, t) = 0$

**Case-2**

- $x = 0$
  - $u_x(x = 0, y, t) = 0$
  - $u_y(x = 0, y, t) = 0$
  - $T(x = 0, y, t) = 0^\circ$ C
  - $\Phi(x = 0, y, t) = 0$ volt

- $x = L$
  - $\sigma_{xx}(x = L, y, t) = 0$
  - $\sigma_{yx}(x = L, y, t) = 0$
  - $T(x = L, y) = 0^\circ$ C
  - $\Phi(x = L, y, t) = 0$ volt

- $y = 0$
  - $\sigma_{yy}(x, y = 0, t) = 0$
  - $\sigma_{xy}(x, y = 0, t) = 0$
  - $T(x, y = 0, t) = 0$
  - $\Phi_y(x, y = 0, t) = 0$

- $y = W$
  - $\sigma_{yy}(x, y = W, t) = 0$
  - $\sigma_{xy}(x, y = W, t) = 0$
  - $T(x, y = W, t) = 0$
  - $\Phi_y(x, y = W, t) = 0$
Comparison of voltage distribution

Peridynamics

FEA
Comparison of temperature distribution

Peridynamics

FEA
Comparison of current density

Peridynamics

FEA
Variation of area $(\mu m)^2$ due to electromigration