FOURIER-solution in Peridynamic (Olaf Weckner)

Mini-Workshop 1103b: Mathematical Analysis for Peridynamics

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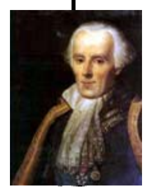
The effect of long-range forces on the dynamics of a bar

Local elasticity

$$\frac{1}{c^2}\partial_t^2 u(x,t) - \partial_x^2 u(x,t) = f(x,t)$$

$$\frac{1}{c^2}\partial_t^2 \bar{u}(k,t) + k^2 \bar{u}(k,t) = \bar{f}(k,t)$$

$$\hat{u}(k,s) = \frac{\hat{f}(k,s)c^2}{s^2+k^2c^2} + \bar{u}(k,+0)\frac{s}{s^2+k^2c^2} + \partial_t \bar{u}(k,+0)\frac{1}{s^2+k^2c^2}$$



Nonlocal elasticity

$$\rho_0 \ddot{u}(x,t) = \int_{\mathcal{R}} C(\xi)\,(u(\xi+x,t)-u(x,t))\,d\xi + b(x,t)$$

$$\ddot{\bar{u}}(k,t) + \omega^2(k)\,\bar{u}(k,t) = \frac{\bar{b}(k,t)}{\rho_0}$$

$$\omega(k) := \sqrt{\frac{\bar{C}(0)-\bar{C}(k)}{\rho_0}}.$$

$$\bar{u}(k,s) = \frac{\hat{b}(k,s)/\rho_0}{\omega^2(k)+s^2} + +\bar{u}(k,+0)\frac{s}{s^2+\omega^2(k)} + \partial_t \bar{u}(k,+0)\frac{1}{s^2+\omega^2(k)}$$

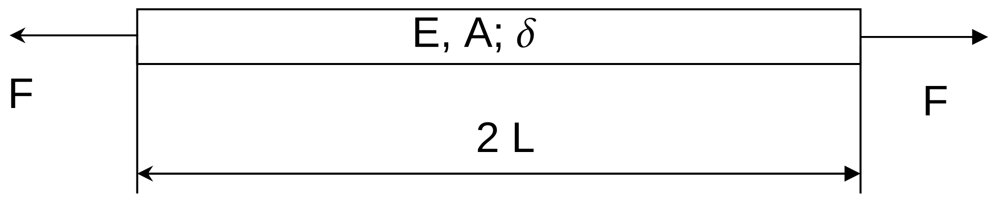
$$\mathcal{L}^{-1}\ \mathcal{F}^{-1}$$

$$\begin{aligned} u(x,t) &= u_p(x,t) + u_h(x,t), \\ u_p(x,t) &= \frac{c}{2}\int_0^t \int_{x-c(t-\hat{t})}^{x+c(t-\hat{t})} f(\hat{x},\hat{t})\,d\hat{x}d\hat{t}, \\ u_h(x,t) &= \frac{u_0(x-ct)+u_0(x+ct)}{2} + \frac{1}{2c}\int_{x-ct}^{x+ct} v_0(\hat{x})\,d\hat{x}. \end{aligned}$$

$$u(x,t) = \int_{-\infty}^{+\infty} u_0(x-\hat{x})\frac{\partial}{\partial t}g(\hat{x},t)\,d\hat{x} + \int_{-\infty}^{+\infty} v_0(x-\hat{x})g(\hat{x},t)\,d\hat{x} + \int_0^t \int_{-\infty}^{+\infty} \frac{b(x-\hat{x},t-\hat{t})}{\rho_0} g(\hat{x},\hat{t})d\hat{x}\,d\hat{t},$$

$$g(x,t) = \mathcal{F}^{-1}\left\{\frac{\sin(\omega(k)\,t)}{\omega(k)}\right\} = \frac{1}{2\,\pi}\int_{-\infty}^{+\infty} e^{ikx}\frac{\sin(\omega(k)\,t)}{\omega(k)}\,dk$$

Static analytical solutions in 1D



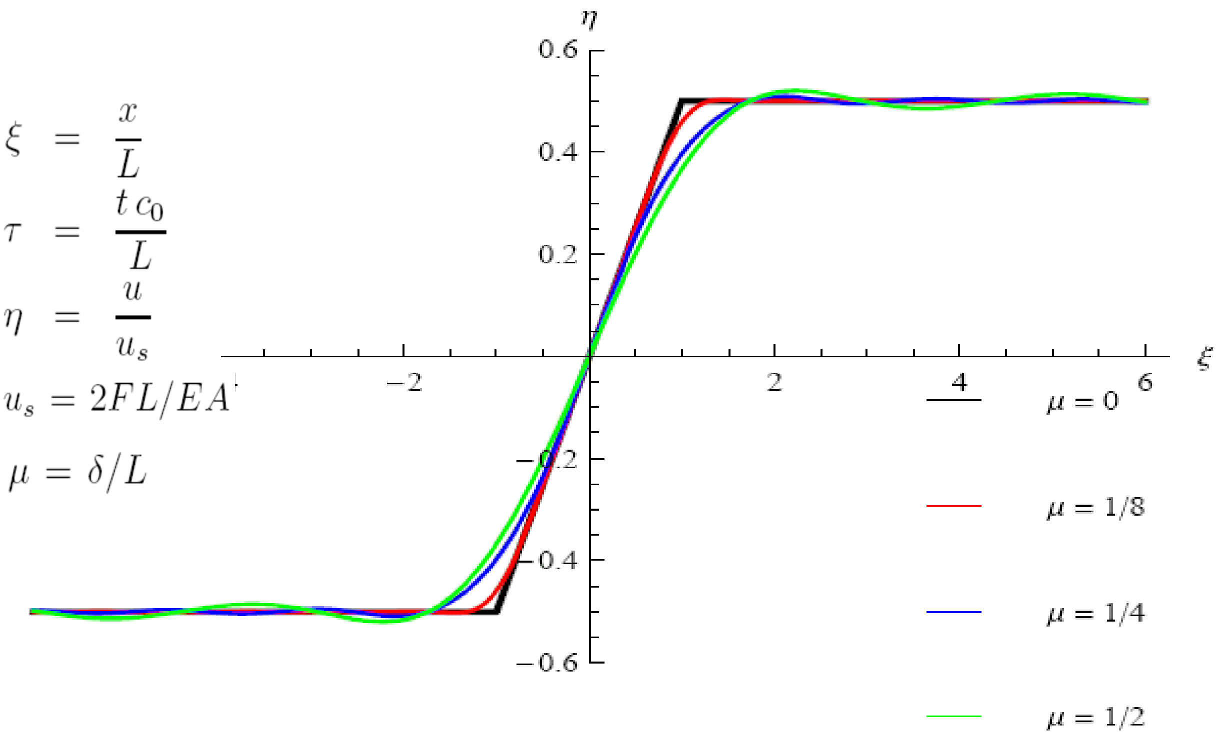
$$\xi = \frac{x}{L}$$

$$\tau = \frac{t\,c_0}{L}$$

$$\eta = \frac{u}{u_s}$$

$$u_s = 2FL/EA$$

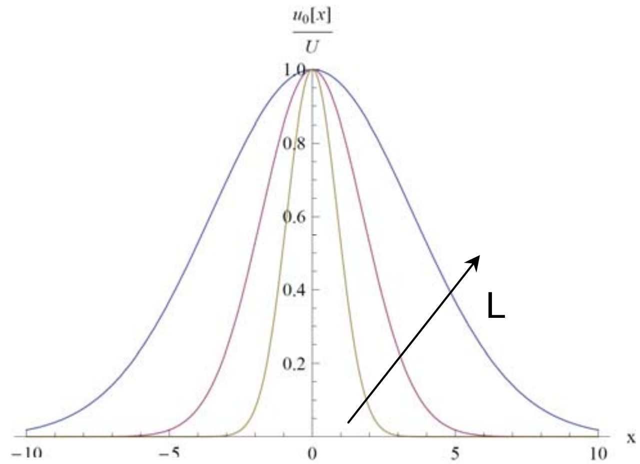
$$\mu = \delta/L$$



The effect of long-range forces on the dynamics of a bar

Example I: Initial value problem

$$
\begin{aligned}
u_0(x) &= U e^{-(x/L)^2} \\
v_0(x) &= 0
\end{aligned}
$$



Normalization $\xi = \frac{x}{L}, \quad \tau = \frac{t\, c_0}{L}, \quad \eta = \frac{u}{U}, \quad \lambda = \frac{\delta}{L}$

Solution

$$
\begin{aligned}
\eta^{local}(\xi, \tau) &= \frac{1}{2}\left(e^{-\left(\frac{\xi-\tau}{2}\right)^2} + e^{-\left(\frac{\xi+\tau}{2}\right)^2} \right) \\
\eta^{nonlocal}(\xi, \tau; \lambda) &= \frac{2}{\sqrt{\pi}} \int_0^\infty \cos(\alpha\xi) e^{-\alpha^2} \cos(\tau \sqrt{\frac{1 - e^{-\alpha^2\lambda^2}}{\lambda^2}}) d\alpha
\end{aligned}
$$

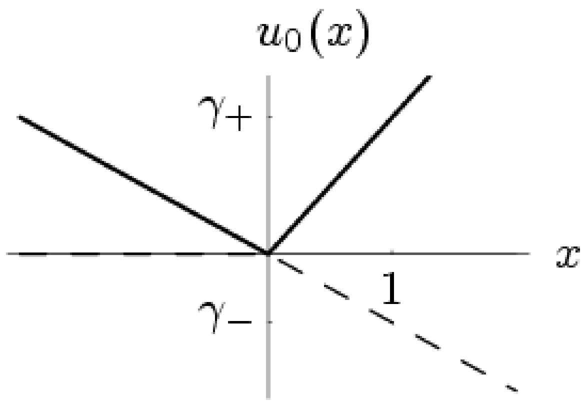
Plots

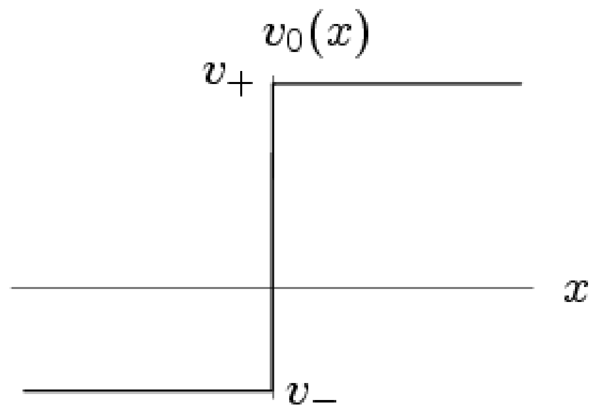
λ= 1 λ= 1/2 λ= 1/8

For δ << L the solutions converge.

Example II: The Riemann-Problem

Initial Conditions





A jump in the velocity field leads to a displacement discontinuity!

Jump Conditions

General Balance (3D)

$$
\begin{aligned}
\frac{d}{dt}\Phi &= \Psi = \Psi_{\mathcal{A}} + \Psi_{\mathcal{V}}, \\
\Phi &= \int_{\mathcal{V}} dV\,\varphi, \\
\Psi_{\mathcal{A}} &= \int_{\partial\mathcal{V}} dA\,\boldsymbol{n}\cdot\psi_{\mathcal{A}}, \\
\Psi_{\mathcal{V}} &= \int_{\mathcal{V}} dV\,\psi_{\mathcal{V}}.
\end{aligned}
$$

Field Equation

$$\partial_t\varphi + \nabla\cdot(\boldsymbol{v}\varphi) = \nabla\cdot\psi_{\mathcal{A}} + \psi_{\mathcal{V}}.$$

Jump Conditions

$$\boldsymbol{n}\cdot[[(\boldsymbol{v}-\mathbf{c})\varphi]] = \boldsymbol{n}\cdot[[\psi_{\mathcal{A}}]].$$

Momentum Balance (1D)

$$[[\dot{u}(s(t),t)]]\dot{s} = 0.$$

Continuity (1D)

$$[[\dot{u}(s(t),t)]] + [[\partial_x u(s(t),t)]]\dot{s} = 0$$

Time-history of displacement jump

Rewrite Equation of Motion $\rho_0 \ddot{u}(x,t) = \int_{-\infty}^{\infty} C(x'-x) \Big(u(x',t) - u(x,t) \Big) \, dx' + b(x,t)$

$$\rho_0 \ddot{u}(x,t) + \bar{C}(0)\, u(x,t) \quad = \quad \int_{-\infty}^{\infty} C(\xi)\, u(\xi + x, t)\, d\xi + b(x,t)$$

with *average stiffness*

$$\bar{C}(0) = \int_{-\infty}^{+\infty} C(\xi) d\xi$$

leads to

$$\rho_0 \partial_t^2 [[u(s,t)]] + \bar{C}(0)[[u(s,t)]] = [[b(s,t)]]$$

with solution

$$[\![u(0,t)]\!] = \triangle_0 u(0,t) = \ell \, \frac{(v_+ - v_-)}{c_0} \, \sin\left(\frac{c_0 t}{\ell}\right)$$

Determination of nonlocal constitutive equations from phonon dispersion relations

Recap: 1D peridynamic equation of motion

$$\rho_0 \ddot{u}(x,t) = \int_{\mathcal{R}} C(\xi)\left(u(\xi + x, t) - u(x,t)\right) d\xi + b(x,t)$$

with solution

$$\begin{aligned} u(x,t) &= \int_{-\infty}^{+\infty} u_0(x-\hat{x})\dot{g}(\hat{x},t)d\hat{x} + \int_{-\infty}^{+\infty} v_0(x-\hat{x})g(\hat{x},t)d\hat{x} \\ &+ \int_0^t \int_{-\infty}^{+\infty} \frac{b(x-\hat{x}, t-\hat{t})}{\rho} g(\hat{x},\hat{t})d\hat{x}d\hat{t} \quad \text{where} \\ g(x,t) &= \mathcal{F}^{-1}\{\frac{\sin(\omega(k)t)}{\omega(k)}\} \equiv \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ikx}\frac{\sin((\omega(k)t)}{\omega(k)}dk \quad \text{and} \\ \omega(k) &= \sqrt{\frac{\bar{C}(0) - \bar{C}(k)}{\rho}} \equiv \left(\int_{-\infty}^{+\infty}(1-\cos(k\xi))C(\xi)d\xi/\rho\right)^{1/2}. \end{aligned}$$

Idea: invert dispersion relation to solve for nonlocal constitutive equation / micromodulus function C(x)

$$C(x) = \bar{C}(0)\Delta(x) - \rho\mathcal{F}^{-1}\{\omega^2(k)\}$$

Determination of nonlocal constitutive equations from phonon dispersion relations

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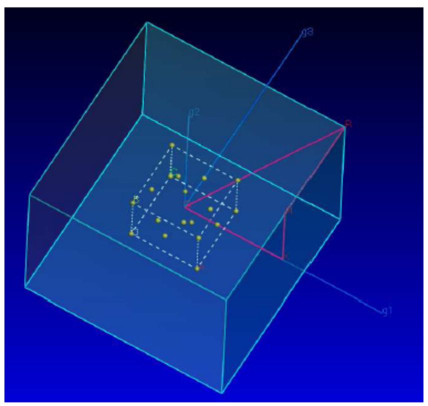
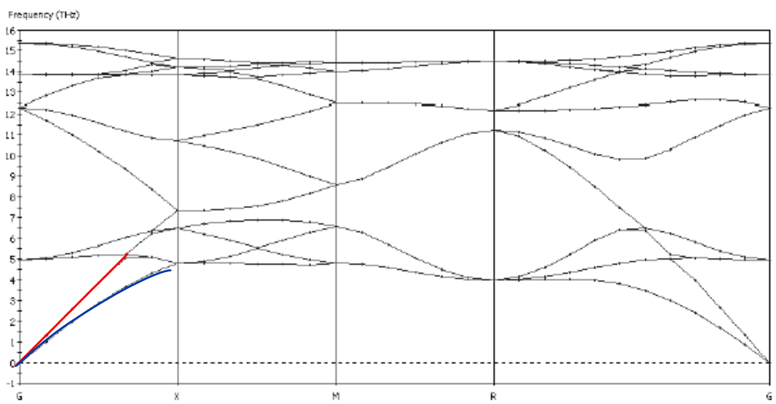
Determine constitutive model for the linear interpolation of a finite set of measured / calculated dispersion data $\omega(k_i) = \omega_i$

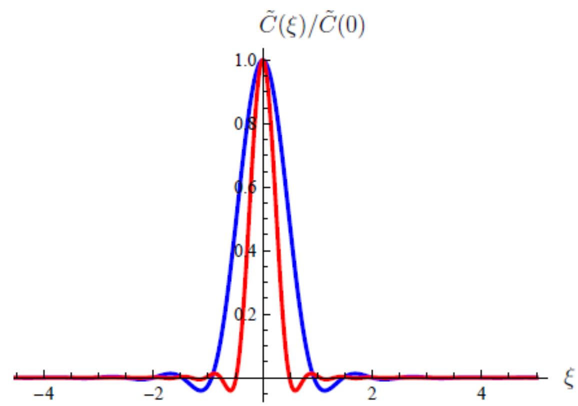
$$\tilde{C}(x) = \frac{\rho}{\pi}\left(\omega_n^2 \frac{\sin(\Delta k n x)}{x} - \sum_{i=0}^{n-1} \int_{i\Delta k}^{(i+1)\Delta k} \cos(kx)\left(\omega_i + \frac{\omega_{i+1}-\omega_i}{\Delta k}(k - i\Delta k)\right)^2 dk\right)$$



Diamond structure of a silicon



: Phonon dispersion relations for silicon calculated with CASTEP



Longitudinal (red) and transverse (blue) micromodulus functions for Si

3D analytical solution using FOURIER transforms

Joseph Fourier
(1768-1830)

Equation of motion in (x,t) space

$$
\begin{aligned}
\rho\, \ddot{\mathbf{u}}(\boldsymbol{x}, t) &= \mathcal{L}[\boldsymbol{u}(\boldsymbol{x}, t)] + \boldsymbol{b}(\boldsymbol{x}, t) \\
{}^{L}\mathcal{L}[\boldsymbol{u}(\boldsymbol{x}, t)] &= (\lambda + \mu)\, \boldsymbol{\nabla}\boldsymbol{\nabla} \cdot \mathbf{u}(\mathbf{x}, \mathbf{t}) + \mu\, \boldsymbol{\nabla} \cdot \boldsymbol{\nabla}\mathbf{u}(\mathbf{x}, \mathbf{t}) \\
{}^{NL}\mathcal{L}[\boldsymbol{u}(\boldsymbol{x}, t)] &= \int_{\mathcal{H}(\boldsymbol{x}, \delta)} \boldsymbol{C}(\boldsymbol{\xi}) \cdot [\boldsymbol{u}(\boldsymbol{x} + \boldsymbol{\xi}, t) - \boldsymbol{u}(\boldsymbol{x}, t)]\, dV_{\xi}
\end{aligned}
$$

$$\boldsymbol{C}(\boldsymbol{\xi}) = \Lambda(\xi)\boldsymbol{\xi}\boldsymbol{\xi}$$

Equation of motion in FOURIER space (k,t)

$$
\begin{aligned}
\rho\, \ddot{\bar{\mathbf{u}}}(\boldsymbol{k}, t) &+ \boldsymbol{M}(\boldsymbol{k}) \cdot \bar{\boldsymbol{u}}(\boldsymbol{k}, t) = \bar{\boldsymbol{b}}(\boldsymbol{k}, t) \\
\boldsymbol{M}(\boldsymbol{k}) &= M_{\|}(k)\boldsymbol{n}_k\boldsymbol{n}_k + M_{\perp}(k)\underbrace{\boldsymbol{I}_{\boldsymbol{n}_k}} \\
{}^{L}M_{\|}(k) &= (\lambda + 2\mu)\; k^2 \\
{}^{L}M_{\perp}(k) &= \mu\; k^2 \\
{}^{NL}M_{\|}(k) &= 4\pi \int_0^{\delta} \Lambda(r) r^4 A_1(kr)\, dr \\
{}^{NL}M_{\perp}(k) &= 4\pi \int_0^{\delta} \Lambda(r) r^4 A_2(kr)\, dr \\
A_1(x) &= \frac{1}{3} - \frac{\sin(x)}{x} - \frac{2\cos(x)}{x^2} + \frac{2\sin(x)}{x^3} = \frac{x^2}{10} + O(x^4) \\
A_2(x) &= \frac{1}{3} + \frac{\cos(x)}{x^2} - \frac{\sin(x)}{x^3} = \frac{x^2}{30} + O(x^4)
\end{aligned}
$$

Projector $\boldsymbol{I}_n = (\boldsymbol{I} - \boldsymbol{n}\boldsymbol{n})$

3D solution using FOURIER transforms

Pierre-Simon Laplace
1749 –1827

Equation of motion in LAPLACE space (k,s)

$$\tilde{\boldsymbol{u}}(\boldsymbol{k}, s) = (\rho s^2 \boldsymbol{I} + \boldsymbol{M}(\boldsymbol{k}))^{-1} \cdot (\tilde{\boldsymbol{b}}(\boldsymbol{k}, s) + s\bar{\boldsymbol{u}}^0(\boldsymbol{k}) + \bar{\boldsymbol{v}}^0(\boldsymbol{k}))$$

$$(\rho s^2 \boldsymbol{I} + \boldsymbol{M}(\boldsymbol{k}))^{-1} = \frac{\boldsymbol{n}_k \boldsymbol{n}_k}{\rho s^2 + M_{\|}(k)} + \frac{\boldsymbol{P}_{\boldsymbol{n}_k}}{\rho s^2 + M_{\perp}(k)}.$$

Applying the inverse transformation gives

$$\begin{aligned}\boldsymbol{u}(\boldsymbol{x}, t) \;=\; & \int_{\mathcal{B}} \boldsymbol{u}^0(\boldsymbol{x} - \hat{\boldsymbol{x}}) \cdot \dot{\boldsymbol{g}}(\hat{\boldsymbol{x}}, t) dV_{\hat{x}} \\ & + \int_{\mathcal{B}} \boldsymbol{v}^0(\boldsymbol{x} - \hat{\boldsymbol{x}}) \cdot \boldsymbol{g}(\hat{\boldsymbol{x}}, t) dV_{\hat{x}} \\ & + \int_{\mathcal{B}} \int_{\mathcal{T}} \frac{\boldsymbol{b}(\boldsymbol{x} - \hat{\boldsymbol{x}}, t - \hat{t})}{\rho} \cdot \boldsymbol{g}(\hat{\boldsymbol{x}}, \hat{t}) d\hat{t} dV_{\hat{x}}\end{aligned}$$

with the GREEN's tensor g

$$\begin{aligned}\boldsymbol{g}(\boldsymbol{x}, t) &= \boldsymbol{I} f_1(x, t) + \boldsymbol{n}_x \boldsymbol{n}_x f_2(x, t) \text{ with} \\ f_1(x, t) &= \frac{1}{2\pi^2} \int_0^\infty k^2 [\, (\frac{1}{3} - A_2(xk)) \left(\frac{\sin(\omega_{\|}(k)t)}{\omega_{\|}(k)} - \frac{\sin(\omega_{\perp}(k)t)}{\omega_{\perp}(k)} \right) + \frac{\sin(kx)}{kx} \frac{\sin(\omega_{\perp}(k)t)}{\omega_{\perp}(k)} \,]\, dk \\ f_2(x, t) &= \frac{1}{2\pi^2} \int_0^\infty k^2 (A_2(xk) - A_1(xk)) \left(\frac{\sin(\omega_{\|}(k)t)}{\omega_{\|}(k)} - \frac{\sin(\omega_{\perp}(k)t)}{\omega_{\perp}(k)} \right) dk\end{aligned}$$

3D solution using FOURIER transforms

Specializing to the static case with $b(x) = P\delta(x)$ we find the solution

$$\begin{aligned}
\boldsymbol{u}(\boldsymbol{x}) &= \mathcal{F}^{-1}\{\boldsymbol{M}^{-1}(\boldsymbol{k})\} \cdot \boldsymbol{P} \quad \text{with} \\
\mathcal{F}^{-1}\{\boldsymbol{M}^{-1}(\boldsymbol{k})\} &= f_{\boldsymbol{n}_x}(x)\boldsymbol{n}_x\boldsymbol{n}_x + f_{\boldsymbol{I}_{\boldsymbol{n}_x}}(x)\boldsymbol{I}_{\boldsymbol{n}_x} \\
f_{\boldsymbol{n}_x}(x) &= \frac{1}{2\pi^2}\int_0^\infty [\, a_1(xk)\left(\frac{k^2}{M_\perp(k)} - \frac{k^2}{M_{||}(k)}\right) + \frac{\sin(kx)}{kx}\frac{k^2}{M_\perp(k)}\,]\, dk \\
f_{\boldsymbol{I}_{\boldsymbol{n}_x}}(x) &= \frac{1}{2\pi^2}\int_0^\infty [\, a_2(xk)\left(\frac{k^2}{M_\perp(k)} - \frac{k^2}{M_{||}(k)}\right) + \frac{\sin(kx)}{kx}\frac{k^2}{M_\perp(k)}\,]\, dk
\end{aligned}$$

Sanity check: local elasticity solution (LOVE 1927)

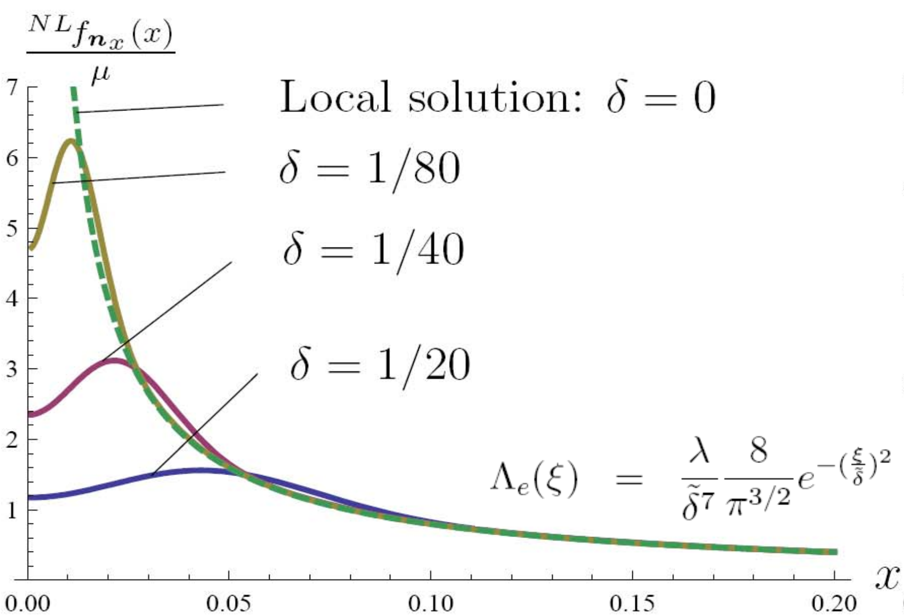
$$^{L}\boldsymbol{u}(\boldsymbol{x}) = \underbrace{\frac{1}{8\pi\mu x}}\left(2\,\boldsymbol{n}_x\boldsymbol{n}_x + \frac{\lambda+3\mu}{\lambda+2\mu}\boldsymbol{I}_{\boldsymbol{n}_x}\right)\cdot\boldsymbol{P}$$

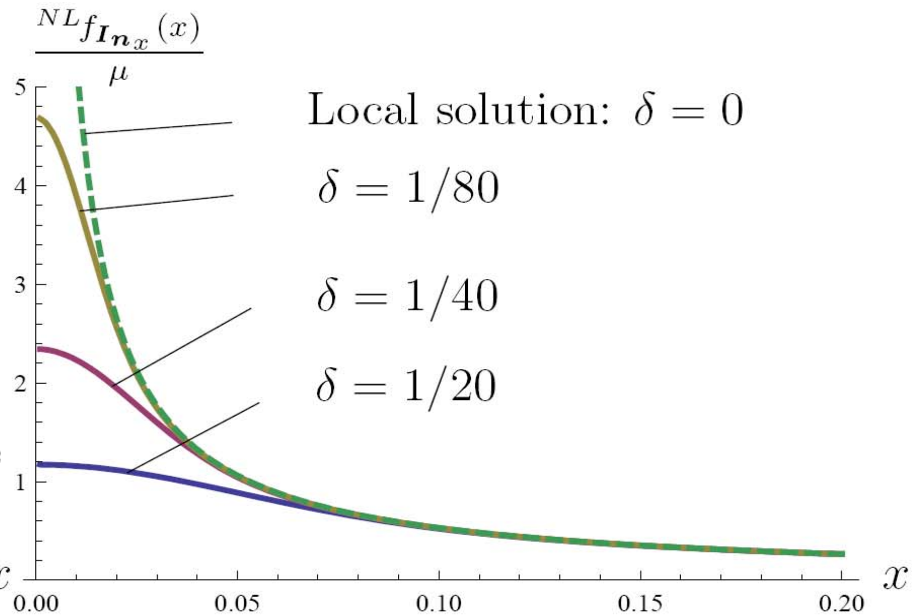
How does this term look like
in non-local elasticity / peridynamics?

Augustus Edward
Hough Love
1863 -1940

3D solution using FOURIER transforms

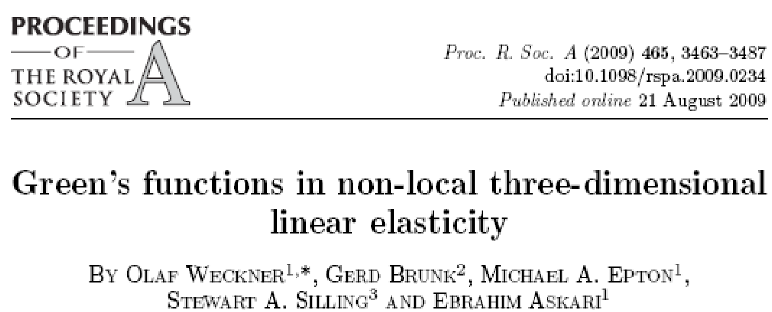
Numerical integration for nonlocal case gives





- The non-local solu … x > 0.
- At x = 0 peridynan …

Nonlocal peridyna … anics and thus avoids the numeri … ds, or a crack tip!



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Green's functions in non-local three-dimensional linear elasticity

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