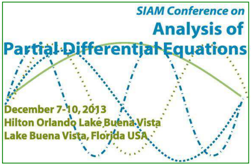
Towards Addressing Surface Effects
Ordinary Isotropic Peridynamic Models
Position Aware Linear Solid (PALS)

SAND2013-10321C

John Mitchell & Stewart Silling

Sandia National Laboratories
Albuquerque, New Mexico

Sandia National Laboratories is a multi-program laboratory managed and operated, by Sandia Corporation a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL8500.



Acknowledgments

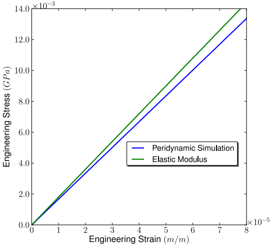
Thanks for the Help and Support

- Dave Littlewood – project support and generally helpful with running and developing within *Peridigm*
- Stewart Silling – PALS concepts, technical support and guidance
- Mike Parks – project support

What is the *Dreaded Surface Effect*?
Example: Isotropic-Ordinary Model

Axial Displacement

Stress versus Strain



Stored Elastic Energy

The following related aspects contribute to the above mismatch.

- Geometric surface effects
- Nonlocal model (dilatation on surface) and model properties
- Discretization error

This talk is about working towards a practical solution.

Ordinary peridynamic models
Dreaded Surface Effect

Key manifestations

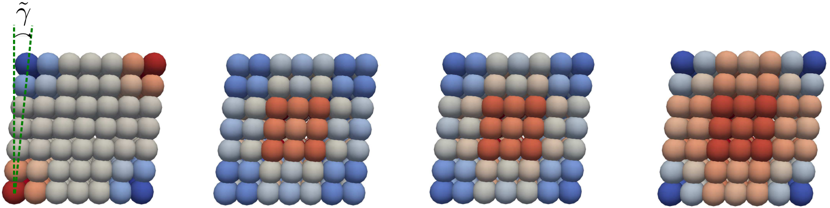
- On simple problems, computed solutions conflict with expectations
- Surface effects *induce* a different boundary value problem

Proposed Corrections

- *DSF*: Position aware scalar correction (March 2013)
- *PALS*: Today's presentation

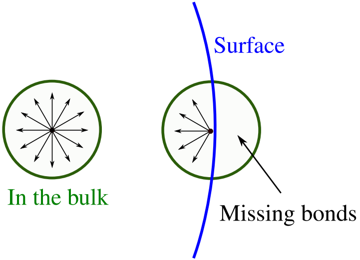
Model Problem

- Simple shear (more later)

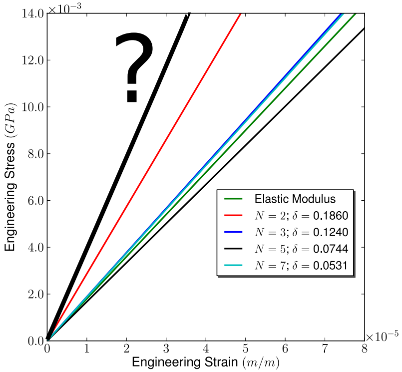


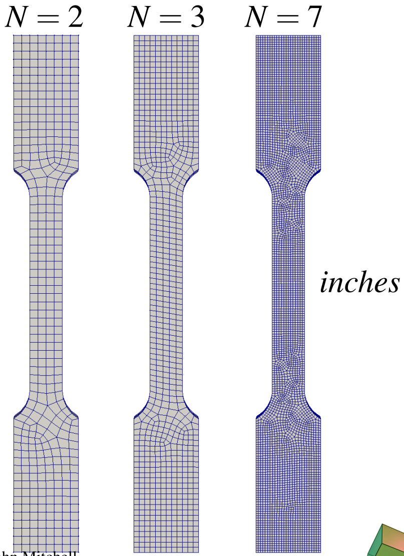
Causes relate to material points near surface

- Mathematical models assume all points are in the *bulk*
  - Points near surface are *missing bonds*
  - *Missing bonds* imply and induce incorrect material properties
  - In the bulk mathematical models are consistent
- Isotropic ordinary materials have a *dilatation defect* at the surface



Mesh Refinement Study
Horizon is tied to mesh element size h: $\delta = 3h$





John Mitchell

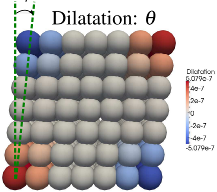
Model problem: simple shear
Ordinary isotropic material model: energy density

Consider simple shear: $u = \tilde{\gamma} y; \quad v = 0; \quad w = 0; W_L = \frac{1}{2}\mu\tilde{\gamma}^2$

$$\mu = 6.923 \times 10^{11}; \quad K = 1.5 \times 10^{12}; \quad \tilde{\gamma} = 1.0 \times 10^{-6}; \quad W_L \approx .34615$$

$\tilde{\gamma}$

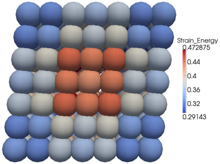
Dilatation: θ



Energy Density: W

$e^d = |\underline{\mathbf{Y}}| - |X| - \frac{\theta}{3}$

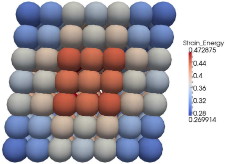
$W = \frac{1}{2}K\theta^2 + \frac{1}{2}\alpha e^d \bullet e^d$



Energy Density: W

$e^d = |\underline{\mathbf{Y}}| - |X|$

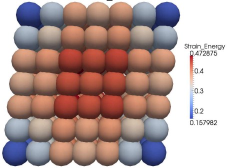
$W = 0 + \frac{1}{2}\alpha e^d \bullet e^d$



Energy Density: W

$e^d = |\underline{\mathbf{Y}}| - |X| - \frac{\theta}{3}$

$W = 0 + \frac{1}{2}\alpha e^d \bullet e^d$



Outline

- Compare models: *LPS* with *PALS*
- Selecting/creating/evaluating influence functions
- *matching deformations*: dilatation, deviatoric
- *Examples*

Isotropic ordinary elastic models
Compare *LPS* with *PALS*

Kinematics

$$e = |\underline{\mathbf{Y}}| - |X| \qquad \underline{\varepsilon} = e - \frac{\theta}{3}|X| \qquad \text{Bond: } \xi = x' - x = X\langle\xi\rangle$$

Linear peridynamic solid model

$$W = \frac{1}{2}K\theta^2 + \frac{\alpha}{2}(\omega\underline{\varepsilon}) \bullet \underline{\varepsilon}, \qquad \theta = \frac{3}{m}(\omega|X|) \bullet e$$

$$m = \omega|X| \bullet |X|, \qquad \alpha = \frac{15\mu}{m}$$

PALS model

$$W = \frac{1}{2}K\theta^2 + \mu(\sigma\underline{\varepsilon}) \bullet \underline{\varepsilon}, \qquad \theta = (\omega|X|) \bullet e$$

Selecting influence functions
Compare *LPS* with *PALS*

Linear peridynamic solid model

- ω is given and used for every point in mesh

PALS model

- ω, σ are computed for each point in mesh
- Initial influence functions ω_0, σ_0 given
- Select ω, σ as best approximations to ω_0,σ_0 subject to kinematic constraints: *matching deformations* $e^k\langle\xi\rangle = \frac{\xi \cdot H^k \xi}{|\xi|}$

$$I(\omega,\lambda^{1:6}) = \frac{1}{2}(\omega-\omega_0)\bullet(\omega-\omega_0) - \sum_{k=1}^{6} \lambda^k(\omega|X|\bullet e^k - Tr(H^k))$$

$$J(\sigma,\tau^{1:6}) = \frac{1}{2}(\sigma-\sigma_0)\bullet(\sigma-\sigma_0) - \sum_{k=1}^{6} \tau^k[(\sigma\varepsilon^k)\bullet\varepsilon^k - |\text{dev symm } H^k|^2]$$

Matching deformations
Probe operator $e^k\langle\xi\rangle = \frac{\xi \cdot H^k \xi}{|\xi|}$

Dilatation

Let probe Δ be denoted by $\Delta = XX = YY = ZZ$

$$\underbrace{\begin{bmatrix} XX & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{H^1} \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & YY & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{H^2} \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & ZZ \end{bmatrix}}_{H^3}$$

Let bond ξ components be denoted by $\{a, b, c\}$

$$e^1 = \frac{\Delta a^2}{|\xi|} \qquad e^2 = \frac{\Delta b^2}{|\xi|} \qquad e^3 = \frac{\Delta c^2}{|\xi|}$$

Matching deformations

Probe operator $e^k\langle \xi \rangle = \frac{\xi \cdot H^k \xi}{|\xi|}$

Deviatoric

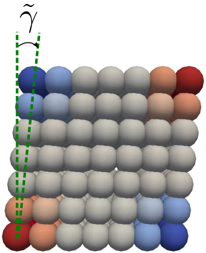
Let probe Δ be denoted by $\Delta = XY = XZ = YZ$

$$\underbrace{\begin{bmatrix} 0 & XY & 0 \\ XY & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{H^4} \underbrace{\begin{bmatrix} 0 & 0 & XZ \\ 0 & 0 & 0 \\ XZ & 0 & 0 \end{bmatrix}}_{H^5} \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & YZ \\ 0 & YZ & 0 \end{bmatrix}}_{H^6}$$

Let bond ξ components be denoted by $\{a, b, c\}$

$$e^4 = \frac{2ab\Delta}{|\xi|} \qquad e^5 = \frac{2ac\Delta}{|\xi|} \qquad e^6 = \frac{2bc\Delta}{|\xi|}$$

Model problem: simple shear
PALS versus *LPS*: expectation *dilatation* $\theta = 0$

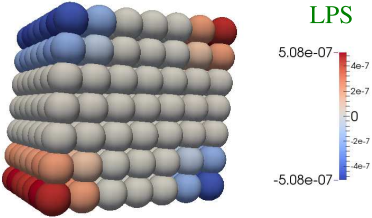


Simple shear

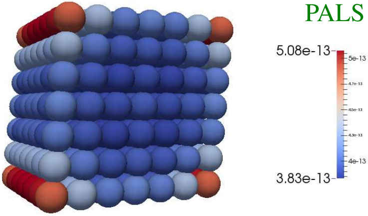
$u = \tilde{\gamma} y; \quad v = 0; \quad w = 0; \quad \tilde{\gamma} = 1.0 \times 10^{-6}$

Dilatation

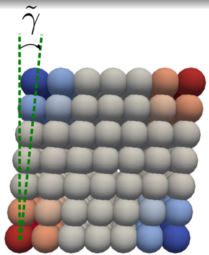
LPS



PALS



Model problem: simple shear
PALS versus *LPS*



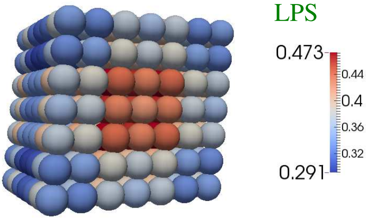
Simple shear

$$u = \tilde{\gamma} y; \quad v = 0; \quad w = 0; \quad \tilde{\gamma} = 1.0 \times 10^{-6}$$

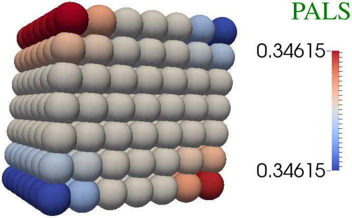
$$W_L = \frac{1}{2}\mu\tilde{\gamma}^2; \quad \mu = 6.923 \times 10^{11}; \quad W_L \approx .34615$$

Stored elastic energy density

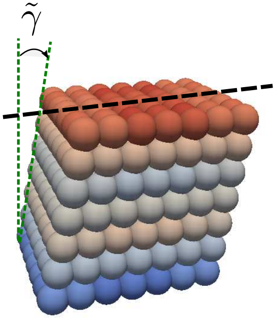
LPS



PALS



Model problem: simple shear
PALS versus *LPS*



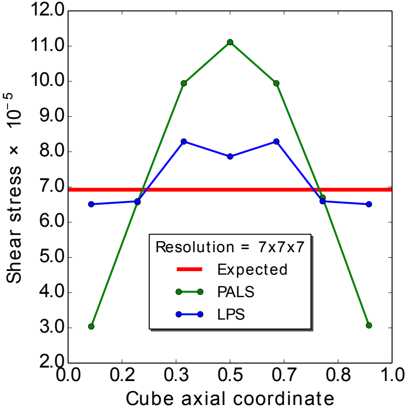
Simple shear *unit cube* $h = \frac{1}{7}$

Shear stress $\sigma_{xy} = \mu\tilde{\gamma} = 6.923 \times 10^5$

$u = \tilde{\gamma}y; \quad v = 0; \quad w = 0; \quad \tilde{\gamma} = 1.0 \times 10^{-6}$

$\mu = 6.923 \times 10^{11}$

Estimated shear stress
$\sigma_{xy} \approx$ *force density* $\times h$



Model problem: simple shear bar
PALS versus *LPS*: Applied deformation

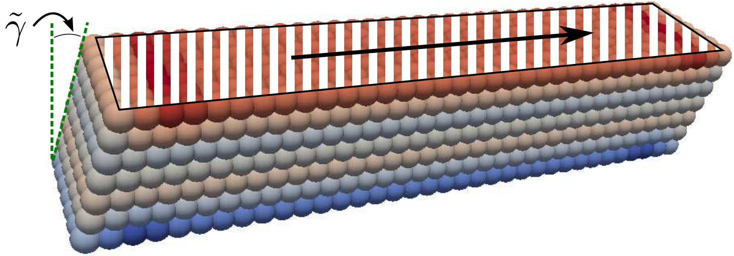
Dimension: $1 \times 1 \times 5$

Mesh resolution: $n_x \times n_y \times n_z = n_x \times n_x \times 5n_x$

Shear stress $\sigma_{xz} = \mu\tilde{\gamma} = 6.923 \times 10^5$

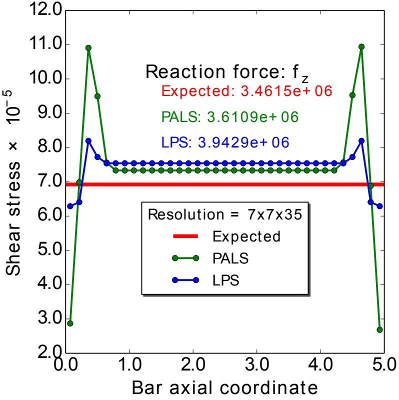
$u = 0; \quad v = 0; \quad w = \tilde{\gamma}y; \quad \tilde{\gamma} = 1.0 \times 10^{-6}$

$f_z = 5 \times \sigma_{xz} \approx 3.4615 \times 10^6$



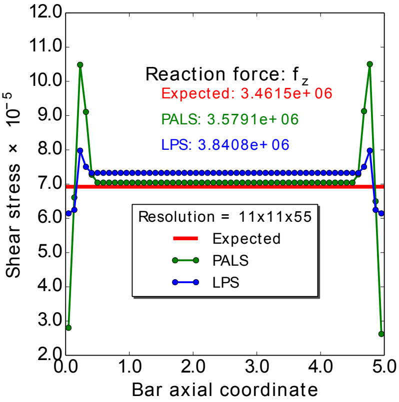
Model problem: simple shear bar
PALS versus *LPS*: Applied deformation

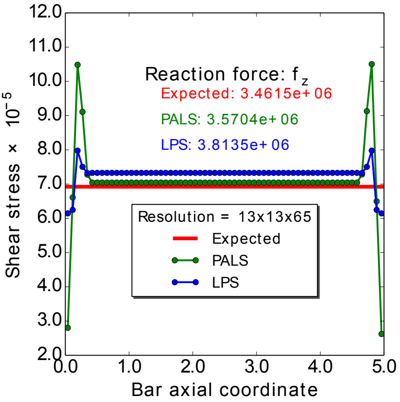
Estimated stress along top surface; Resultant force



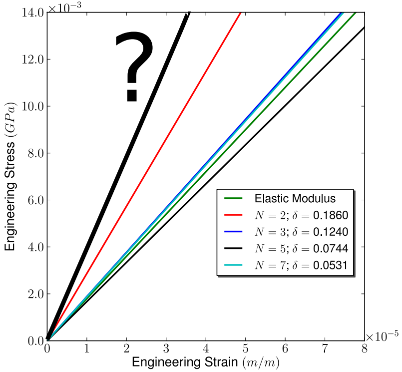
Model problem: simple shear bar
PALS versus *LPS*: Applied deformation

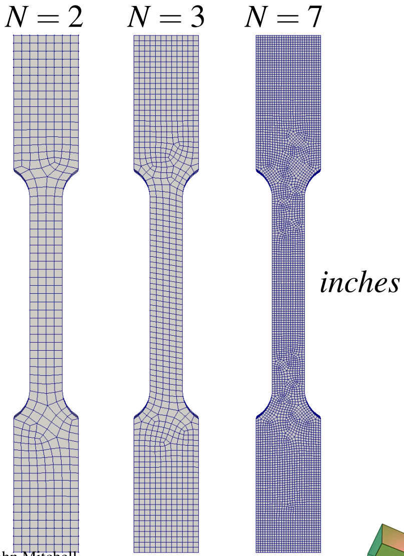
Estimated stress along top surface; Resultant force





Mesh Refinement Study
Horizon is tied to mesh element size h: $\delta = 3\,h$

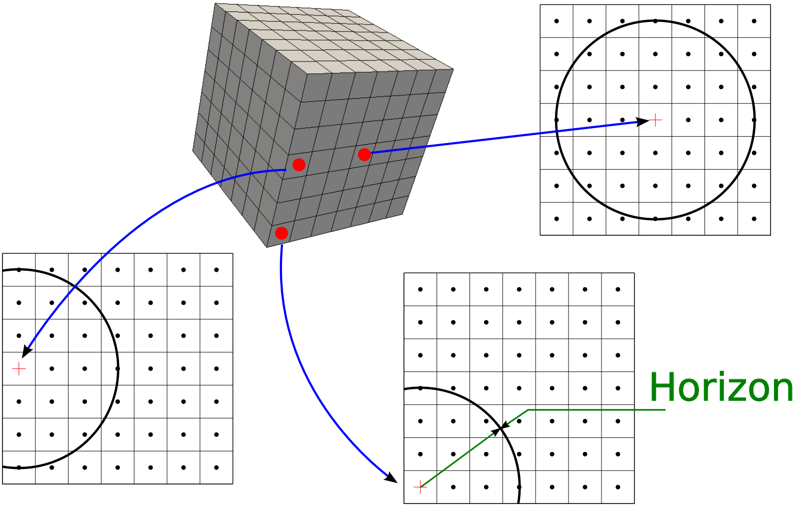




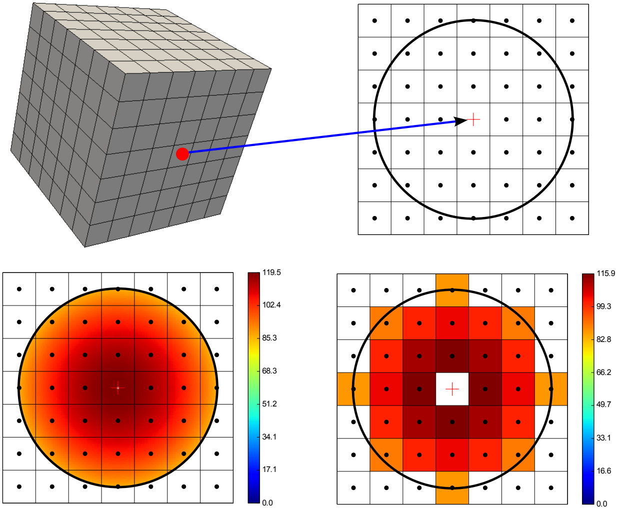
John Mitchell

Sandia National Laboratories

What do the *Pals* influence functions look like?

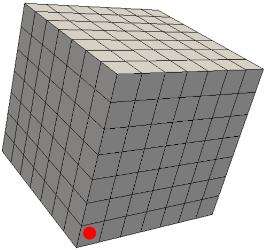


Pals dilatation influence function

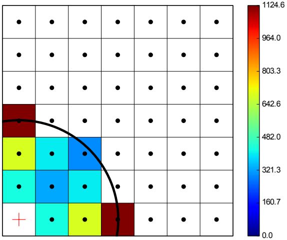


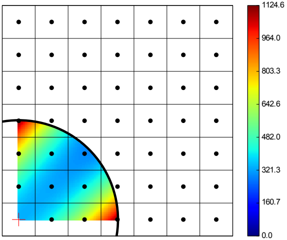
Smooth   Mesh

Pals dilatation influence function

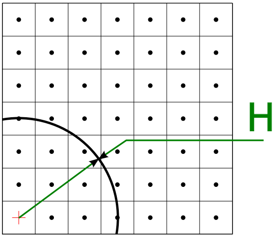


Mesh



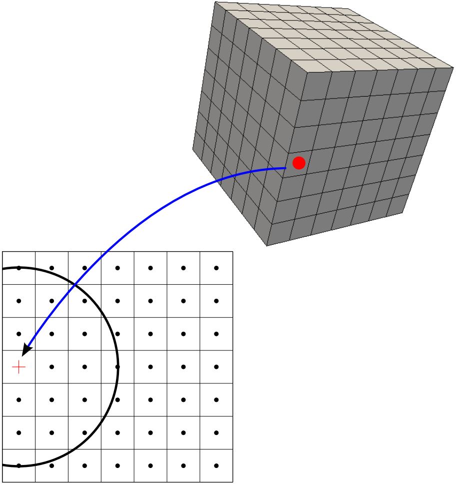


Smooth

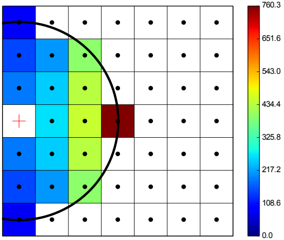


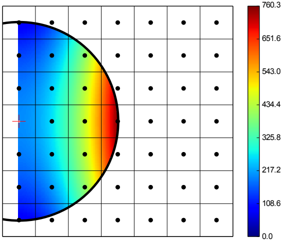
Horizon

Pals dilatation influence function



Mesh





Smooth