On the 'DSF' and the 'Dreaded Surface Effect' SAND2013-1927C

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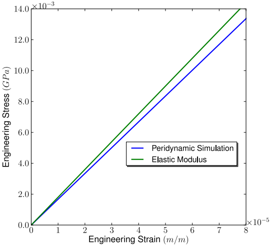
What is the DSF?
For Isotropic-Ordinary Materials
It *MIGHT* be a Practical Solution to the Following Problem

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

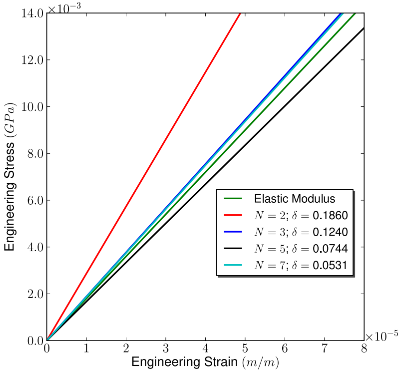
This talk is about working towards a simple/practical solution.

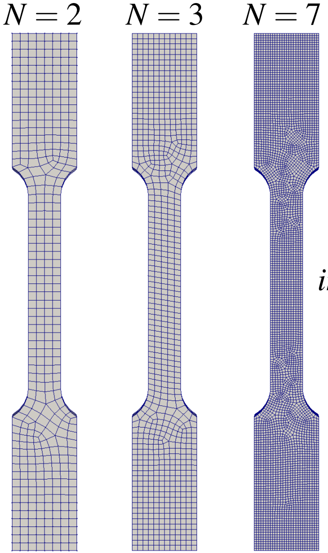
Acknowledgements

Thanks for the Help and Support

- Dave Littlewood – generally helpful with running *Peridigm* and especially for providing the demonstration problem
- Stewart Silling – discussion about the 'DSF' and approach presented here today.
- Mike Parks – *Peridigm* support

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





inches

Review of Isotropic-Ordinary Materials

Scalar Force State $\quad t = \frac{3K\theta}{m}\omega|\xi| + \alpha\omega e^d$

$$e = |Y| - |\xi| \qquad \theta = \frac{3}{m}(\omega|\xi|) \bullet e \qquad e^d = |Y| - |\xi| - \frac{\theta}{3}|\xi|$$

Substituting the above relations

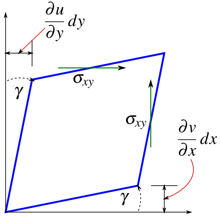
$$t = \left(\frac{3K}{m} - \frac{\alpha}{3}\right)\theta\omega|\xi| + \alpha\omega e$$

If we use $\alpha = \frac{15\mu}{m}$ (trouble starts here)

$$t = \left(\frac{9K - 15\mu}{3m}\right)\theta\omega|\xi| + \alpha\omega e$$

We need a 'discretization' appropriate and 'geometric' appropriate α

infinitesimal shear deformation St. Venant-Kirchhoff Material



Displacements

$$\begin{aligned} u &= \gamma y \\ v &= \gamma x \\ w &= 0 \end{aligned}$$

Deformation Gradient F

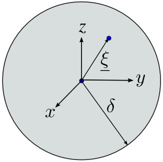
$$[F] = \begin{bmatrix} 1 & \gamma & 0 \\ \gamma & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

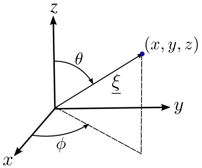
Green Lagrange-Strain E

$$\begin{aligned} 2[E] &= [F]^t[F] - I \\ &= \begin{bmatrix} \gamma^2 & 2\gamma & 0 \\ 2\gamma & \gamma^2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{aligned}$$

Strain energy density $W_L = \frac{1}{2}\lambda [tr(E)]^2 + \mu E : E = \frac{1}{2}\lambda\gamma^4 + 2\mu\gamma^2$

On a sphere





Deformation State Y

$$Y(\gamma) = \sqrt{z^2 + (y+\gamma x)^2 + (x+\gamma y)^2}$$

Linearize deformation state

$$Y(\gamma) \approx \ldots + \mathcal{O}(\gamma^2)$$

Form extension state e=$Y - |\xi|$

$$e = \gamma |\xi| sin^2(\theta)\sin(2\phi)$$

Verify dilatation is zero

$$\frac{3}{m}|\xi| \bullet e = 0$$

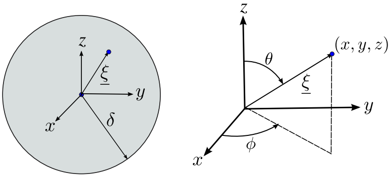
Weighted volume on a sphere

$$m = \frac{4\pi\delta^5}{5}$$

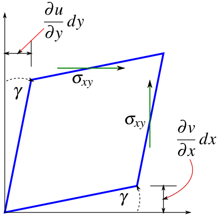
Energy density $W = \frac{1}{2}\alpha e^d \bullet e^d = 2\alpha\frac{m\gamma^2}{15}$

Equating nonlocal W with local W_L

On a sphere



$$W = \frac{1}{2}\alpha e^d \bullet e^d = 2\alpha\frac{m\gamma^2}{15}$$



$$W_L \approx \mu\gamma^2$$

$$W_L = W \implies \alpha = \frac{15\mu}{m}$$

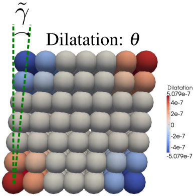
Observations

- W_L is independent of position, i.e., *constant*
- W depends upon neighborhood through integral.

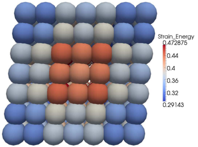
Consider simple shear: $u = \tilde{\gamma} y; \;\; v = 0; \;\; w = 0; \gamma = \frac{\tilde{\gamma}}{2}; \;\; W_L = \frac{1}{2}\mu\tilde{\gamma}^2$

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

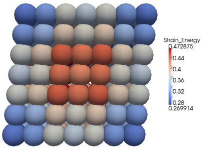
Dilatation: θ



Energy Density: W
$e^d = |Y| - |\xi| - \frac{\theta}{3}$
$W = \frac{1}{2}K\theta^2 + \frac{1}{2}\alpha e^d \bullet e^d$



Energy Density: W
$e^d = |Y| - |\xi|$
$W = 0 + \frac{1}{2}\alpha e^d \bullet e^d$



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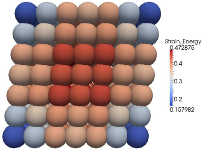


Motivated by Stewart's Approach
Create a Surface Correction Factor: *DSF*

Reconsider elastic energy density for shear at a point

$$W = \frac{1}{2}\tilde{\alpha}||e^d||_h^2 = W_L = 2\mu\gamma^2$$

Divide both sides by $||e^d||^2 = \frac{4m\gamma^2}{15}$, where $m = \frac{4\pi\delta^5}{5}$

$$\begin{aligned}\tilde{\alpha} &= \frac{||e^d||^2}{||e^d||_h^2}\frac{15\mu}{m} \\ &= \frac{4m}{15}\frac{\gamma^2}{||e^d||_h^2}\frac{15\mu}{m} \\ &= DSF \times \alpha\end{aligned}$$

Reconsider Simple Shear Example Using *DSF*

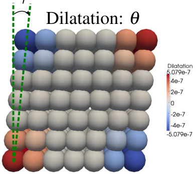
Consider simple shear: $u = \tilde{\gamma} y; \quad v = 0; \quad w = 0; \gamma = \frac{\tilde{\gamma}}{2}; \quad W_L = \frac{1}{2}\mu\tilde{\gamma}^2$

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

$$\alpha = \frac{15\mu}{m}; \quad \tilde{\alpha} \quad = \quad DSF \times \alpha$$

$\tilde{\gamma}$

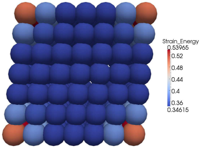
Dilatation: θ



Energy Density: W

$e^d = |Y| - |\xi| - \frac{\theta}{3}$

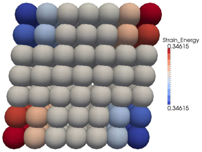
$W = \frac{1}{2}K\theta^2 + \frac{1}{2}\tilde{\alpha}e^d \bullet e^d$



Energy Density: W

$e^d = |Y| - |\xi|$

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



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$e^d = |Y| - |\xi| - \frac{\theta}{3}$

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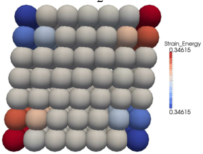
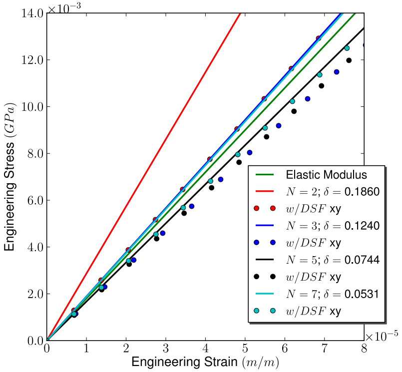
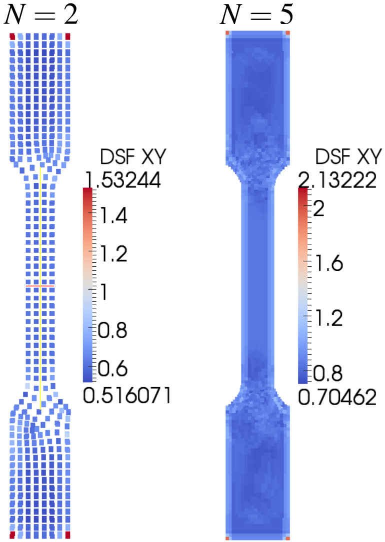


Mesh Refinement Study w/DSF
Horizon is tied to mesh element size h: $\delta = 3\,h$





Algorithm for computing the *DSF*
For all points *XP* in the neighborhood of *X*

Apply pure shear deformation

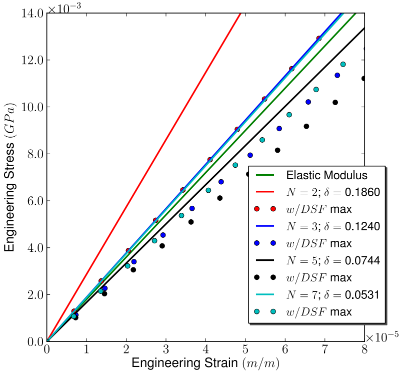
```
double dx = XP[0]-X[0];
double dy = XP[1]-X[1];
double dz = XP[2]-X[2];
double zx(0.0), xy(0.0), yz(0.0);
double xz(0.0), yx(0.0), zy(0.0);
switch(mode){
case ZX:
        zx = gamma * dx;
        xz = gamma * dz;
        break;
case XY:
        xy = gamma * dy;
        yx = gamma * dx;
        break;
case YZ:
        yz = gamma * dz;
        zy = gamma * dy;
        break;
}
YP[0] = XP[0] + xy + xz;
YP[1] = XP[1] + yz + yx;
YP[2] = XP[2] + zx + zy;
```

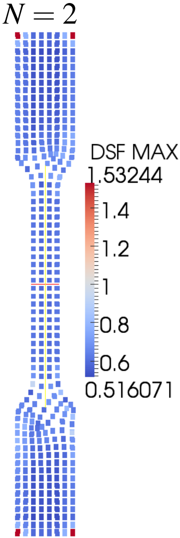
Compute *DSF*

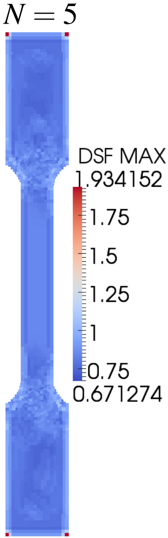
```
double scf, max_dsf, DSF;
int mode = XY;
Y[0] = X[0]; Y[1] = X[1]; Y[2] = X[2];
apply_pure_shear(X,Y,XP,YP,mode,gamma);
scf=ed_squared(neigh[X],X,Y,mode);
max_dsf=scf;

mode = ZX;
Y[0] = X[0]; Y[1] = X[1]; Y[2] = X[2];
apply_pure_shear(X,Y,XP,YP,mode,gamma);
scf=ed_squared(neigh[X],X,Y,mode);
if(scf>max_dsf) max_dsf=scf;

mode = YZ;
Y[0] = X[0]; Y[1] = X[1]; Y[2] = X[2];
apply_pure_shear(X,Y,XP,YP,mode,gamma);
scf=ed_squared(neigh[X],X,Y,mode);
if(scf>max_dsf) max_dsf=scf;

scf=max_dsf;
DSF = 4.0 * gamma * gamma  * m / scf /15.0;
```

Computation on right uses *max*

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







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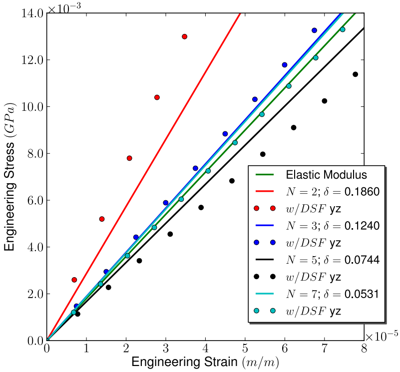

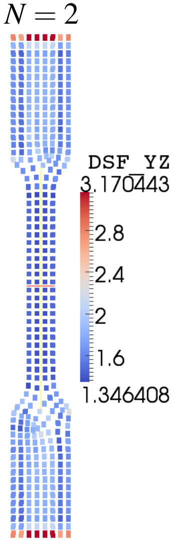

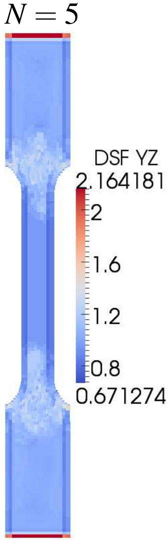

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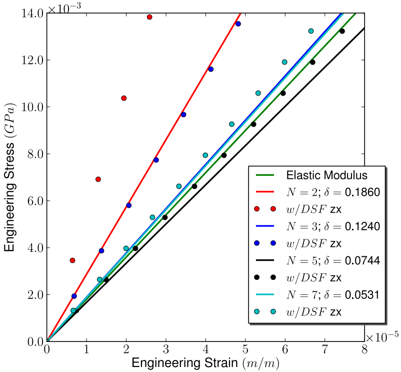

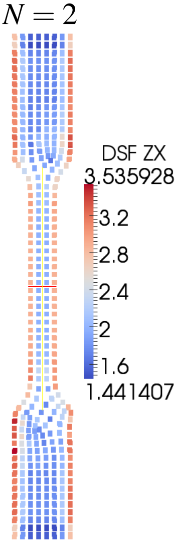

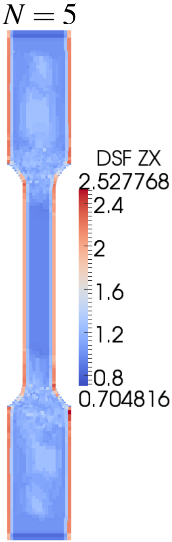

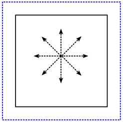

Displacements

$$
\begin{aligned}
u &= \Delta x \\
v &= \Delta y \\
w &= \Delta z
\end{aligned}
$$

Deformation Gradient F

$$
[F] = \begin{bmatrix} 1+\Delta & 0 & 0 \\ 0 & 1+\Delta & 0 \\ 0 & 0 & 1+\Delta \end{bmatrix}
$$

Green Lagrange-Strain E

$$
\begin{aligned}
2[E] &= [F]^t[F] - I \\
&= \begin{bmatrix} \Delta^2+2\Delta & 0 & 0 \\ 0 & \Delta^2+2\Delta & 0 \\ 0 & 0 & \Delta^2+2\Delta \end{bmatrix}
\end{aligned}
$$

Infinitesimal assumption: retain only Δ^2 terms

Strain energy density $W_L = \frac{1}{2}\lambda[tr(E)]^2 + \mu E : E = \frac{1}{2}(9\lambda + 6\mu)\Delta^2$

Closing Remarks and Summary

Expectation for isotropic ordinary materials

- Recover *Youngs Modulus* on a relatively coarse mesh

Using an energy based approach

- Developed shear modulus correction that shows promise
- Speculate that practical/ideal 'DSF' exists
- Question: Is the ideal 'DSF' *anisotropic* at the surface?

Identified issue

- Nonzero dilatation on surface under conditions of pure shear

Surface effect diminishes with mesh refinement

- Convergence is slow but apparent
- On *tensile test*, rate of convergence is inadequate