Today, we will address the last (for now...) challenge associated with quasistatic <u>robust</u> simulation of nonlinear materials $\Rightarrow$ the <u>positive-definiteness</u> of the stiffness matrix K (or lack there of)

<u>Remember</u>: We are using Newton's method to find the minimum-energy configuration for the function $E(\underline{x})$. We do so by iterating

$\underline{x}_{(0)} \leftarrow$ init. guess

for $k = 0, 1, \ldots$

$$\left| \begin{array}{ll} \text{Solve} & -\left.\frac{\partial \underline{f}_{el}}{\partial \underline{x}}\right|_{\underline{x}_{(k)}} \cdot \delta \underline{x} = \underline{f}_{el}(\underline{x}_{(k)}) \quad (1) \\ \text{Update} & \underline{x}_{(k+1)} = \underline{x}_{(k)} + \delta \underline{x} \end{array} \right.$$

where eq (1) can also be seen as

$$K(\underline{x}_{(k)})\, \delta \underline{x} = \underline{f}_{el}(\underline{x}_{(k)}) \quad (2)$$

or even

$$\left.\frac{\partial^2 E}{\partial \underline{x}^2}\right|_{\underline{x}_{(k)}} \cdot \delta \underline{x} = -\left.\frac{\partial E}{\partial \underline{x}}\right|_{\underline{x}_{(k)}} \quad (3)$$

Our problem is that the matrix $K(\underline{x})$ is <u>not</u> guaranteed to be positive definite for <u>any</u> $\underline{x}$

Quiz:

⇒ What would be an example of a configuration $\underline{x}$ where $K(\underline{x})$ would be <u>expected</u> to be indefinite

⇒ Would you expect $K(\underline{x}_{(k)})$ to be positive-definite for a "late" iteration, where $\underline{x}_{(k)}$ is almost converged and why? (or why not?)

The general philosophy behind our remedy:

⇒ Replace the stiffness matrix $K(\underline{x}_{(k)})$ with a <u>modified</u> version $\hat{K}(\underline{x}_{(k)})$ which <u>is</u> designed to be positive-definite (CG can be used!)

⇒ The method becomes <u>modified Newton</u>, iterating

$$\hat{K}(\underline{x}_{(k)})\,\delta\underline{x} = f_{el}(\underline{x}_{(k)})$$

But *why* is this a reasonable remedy?

⇒ It depends on the nature of the modification ($\hat{K}$) but we can say the following:

→ For the specific method we will see, *practice* shows that modified Newton is very robust, especially when combined with inversion-robust fixes (truncating singular values to small positive).

→ Once the modified iteration is close enough to convergence (enough for $K(\underline{x})$ to be s.p.d) we can show that

$$\rho\left(I - [\hat{K}(x_{(k)})]^{-1} K(x_{(k)})\right) < 1$$

spectral radius

then the modified Newton process is guaranteed to converge to the actual minimum.

(i.e. if we are almost converged, a *small* modification does not compromise the ability to converge all the way)

(In-class discussion: 2D nonzero-restlength spring

$$E(\vec{x}) = \frac{k}{2}\left(\|\vec{x} - \vec{x}_0\| - l_0\right)^2$$

)

Outline of the modification

⇒ Split the stiffness matrix to the contribution of individual elements

$$K(\underline{x}) = \sum_{e:\,\text{element}} K^{e}(\underline{x})$$

Each K^{e} corresponds to the contribution of just the e-th element to the energy, i.e:

if $E(\underline{x}) = \sum_{e} E^{e}(x)$

then $K^{e} := -\dfrac{\partial E^{e}(\underline{x})}{\partial \underline{x}}$

if (i, j, k, l) are the vertex indices, then only the blocks of K^{e} corresponding to row/column blocks $i/j/k/l$ will be nonzero

$$K_e = \begin{array}{c} \left[\begin{array}{cccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \times & & \times & & \times & & \times \\ 0 & & 0 & & & & & \\ 0 & \times & & \times & & \times & & \times \\ 0 & & & & 0 & & & \\ 0 & \times & & \times & & \times & & \times \\ 0 & & & & & & 0 & \\ 0 & \times & & \times & & \times & & \times \end{array}\right] \\ \begin{array}{cccccccc} & \uparrow & & \uparrow & & \uparrow & & \uparrow \\ & i & & j & & k & & l \end{array} \end{array}$$

Each "x" is a 3x3 matrix, so, effectively K_e is a 12x12 matrix padded by zeroes to become full-size

⇒ The prescription for the remedy, then, becomes:

⇝ "Project" each elemental stiffness matrix to its positive definite part

$$K^e = Q \Lambda Q^T$$

only 12 of the λ_i's can be nonzero

(in fact, just 9 of them maximum ... why?)

If we define $(\hat{\Lambda})_{ii} = \begin{cases} (\Lambda)_{ii} & , \text{if } \Lambda_{ii} \geq 0 \\ 0 & , \text{if } \Lambda_{ii} < 0 \end{cases}$

and $\hat{K}^e := Q \hat{\Lambda} Q^T$

⇝ Construct the "global" modified stiffness by assembly:

$$\hat{K} := \sum_e \hat{K}^e$$

(some textbooks use an "assembly" operator $\mathcal{A}$ to write $\hat{K} := \underset{e}{\mathcal{A}} \hat{K}^e$

where $\hat{K}^e$ are 12x12 matrices)

If we were prepared to pay the cost of a 12x12 eigenanalysis (9x9, with some effort...) this concludes our fix! (in some cases, we would have no other option).

There is, however, a <u>shortcut</u> to computing <u>exactly</u> the same result, with <u>much reduced cost</u> in the case of <u>isotropic</u> materials (those where $\Psi = \Psi(\Sigma)$)

Implementation

Remember the matrix-free computation of the differential $\delta f[x; \delta x]$

```
addForceDifferential
    foreach element e : (i, j, k, l)
        D_s^e, F^e  <- as before
        δD_s^e, δF^e <- as before
        [ δP^e = δP[F^e; δF^e] ]
        δH^e <- - Vol_e · δP^e (D_m^e)^{-T}
        δH^e -> δf_{i,j,k,l} as before
```

<u>Definiteness fix</u>

Replace $\delta P[F; \delta F]$ with <u>modified</u> $\delta \hat{P}[F; \delta F]$ (next page)

And, here is the prescription for the modified "stress differential"

(Proofs: Teran et al '05 "Robust Quasistatics and Flesh Simulation", SCA '05
Stomakhin et al '12 "Energetically Consistent Invertible Elasticity", SCA '12)

Definitions

$$\mathrm{vec}\left[\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}\right] = \begin{pmatrix} a_{11} \\ a_{22} \\ a_{33} \\ a_{12} \\ a_{21} \\ a_{13} \\ a_{31} \\ a_{23} \\ a_{32} \end{pmatrix}$$

$$\mathrm{mat}\left[\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \\ a_7 \\ a_8 \\ a_9 \end{pmatrix}\right] = \begin{pmatrix} a_1 & a_4 & a_6 \\ a_5 & a_2 & a_8 \\ a_7 & a_9 & a_3 \end{pmatrix}$$

We can show that $\delta P = U\,\mathrm{mat}\left[T \cdot \mathrm{vec}(U^T \delta F V)\right] V^T$

$(F = U \Sigma V^T)$

Where $T = \begin{bmatrix} \underset{(3\times3)}{A} & & & \\ & \underset{(2\times2)}{B_{12}} & & \\ & & \underset{(2\times2)}{B_{13}} & \\ & & & \underset{(2\times2)}{B_{23}} \end{bmatrix}$

where $$A_{ij} = \frac{\partial^2 \psi}{\partial \sigma_i \partial \sigma_j}$$

$$B_{ij} = \frac{1}{2} \frac{\partial\psi/\partial\sigma_i - \partial\psi/\partial\sigma_j}{\sigma_i - \sigma_j} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$+ \frac{1}{2} \frac{\partial\psi/\partial\sigma_i + \partial\psi/\partial\sigma_j}{\sigma_i + \sigma_j} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$