# 14 - finite element method - density growth - theory



14 – density growth

# homework III - revise your final project

due 03/01/12, 09:30am, 300-020

Late homework can be dropped off in a box in front of Durand 217. Please mark clearly with date and time @drop off. We will take off 1/10 of points for each 24 hours late, every 12pm after due date. This homework will count 10% towards your final grade.

#### problem 1 - growth tensors

We have introduced different growth tensors  $F^g$  in class. Discuss the following growth tensors.

1.1 
$$F^{g} = \vartheta I$$

1.2 
$$\mathbf{F}^{\mathrm{g}} = \mathbf{I} + [\vartheta - 1] f_0 \otimes f_0$$

1.3 
$$\mathbf{F}^{\mathrm{g}} = \mathbf{I} + [\vartheta - 1] \mathbf{s}_0 \otimes \mathbf{s}_0$$

1.4 
$$F^g = \sqrt{\vartheta} I + [1 - \sqrt{\vartheta}] n_0 \otimes n_0$$

### homework #03

| day                       | date |    | topic  |  |  |  |
|---------------------------|------|----|--|--|--|--|
| tue                       | jan  | 10 | motivation - everything grows!                       |  |  |  |
| thu                       | jan  | 12 | basics maths - notation and tensors                  |  |  |  |
| tue                       | jan  | 17 | basic kinematics - large deformation and growth      |  |  |  |
| thu                       | jan  | 19 | kinematics - growing hearts                          |  |  |  |
| tue                       | jan  | 24 | guest lecture - growing skin                         |  |  |  |
| thu                       | jan  | 26 | guest lecture - growing leaflets                     |  |  |  |
| tue                       | jan  | 31 | basic balance equations - closed and open systems    |  |  |  |
| thu                       | feb  | 02 | basic constitutive equations - growing tumors        |  |  |  |
| tue                       | feb  | 07 | volume growth - finite elements for growth           |  |  |  |
| hu                        | feb  | 09 | volume growth - growing arteries                     |  |  |  |
| tue                       | feb  | 14 | volume growth - growing skin                         |  |  |  |
| thu                       | feb  | 16 | volume growth - growing hearts                       |  |  |  |
| tue feb 21 basic constitu |      | 21 | basic constitutive equations - growing bones         |  |  |  |
| thu                       | feb  | 23 | density growth - finite elements for growth          |  |  |  |
| tue                       | feb  | 28 | density growth - growing bones                       |  |  |  |
| thu                       | mar  | 01 | everything grows! - midterm summary                  |  |  |  |
| tue                       | mar  | 06 | midterm  |  |  |  |
| hu                        | mar  | 08 | remodeling - remodeling arteries and tendons         |  |  |  |
| tue                       | mar  | 13 | class project - discussion, presentation, evaluation |  |  |  |
| thu                       | mar  | 15 | class project - discussion, presentation, evaluation |  |  |  |
| thu                       | mar  | 15 | written part of final projects due                   |  |  |  |

#### where are we???

#### problem 2 - growth tensors

Assume the following microstructural vectors,  $f_0 = [1, 0, 0]^t$ ,  $s_0 = [0, 1, 0]^t$ , and  $n_0 = [0, 0, 1]^t$  aligned with the cartesian coordinates, and a growth multiplier of  $\theta = 2$ .

- 2.1 Calculate the four growth tensors  $F^g$  from 1.1 to 1.4.
- 2.2 Calculate the volume change of a cube of unit length for all four growth tensors  $F^g$  from 1.1 to 1.4 using the Jacobian  $J^g = \det(F^g)$ .
- 2.3 Draw a cubic block of tissue of unit length in a three-dimensional coordinate system. Add the unit vectors  $dX_1 = [1,0,0]^t$ ,  $dX_2 = [0,1,0]^t$ , and  $dX_3 = [0,0,1]^t$ . For each of the growth tensors  $F^g$  in 1.1 to 1.4, calculate and illustrate the deformed vectors  $dx_1$ ,  $dx_2$  and  $dx_3$  using  $dx = F^g \cdot dX$ . Illustrate the grown block.

### homework #03

#### problem 3 - growing bones in matlab

Last year's class paper "Computational modeling of bone density profiles in response to gait: a subject-specific approach" by Henry Pang, Abhishek Shiwalkar, Chris Madormo, and Rebecca Taylor describes bone growth in the tibia. Read the paper carefully.

- 3.1 Download the matlab file package ME337\_MATLAB.tar.gz from the coursework website or from our lab website http://biomechanics.stanford.edu.
- 3.2 To run the example from the class paper, open the main file nlin\_fem.m in your matlab editor, and make sure that all input file readings are commented out by a % sign in the first column of lines 6 through 22. The only active input line should be line 10 ex henry.

For this part of the homework, it is okay to work in groups, especially if you are not very familiar with matlab. If you create the results in a group, however, the results, interpretations, and discussions must be written individually by each group member. Each group member must understand the matlab algorithm.

#### homework #03

#### balance equations for open systems - mass

$$D_t \rho_0 = \text{Div}(\mathbf{R}) + \mathcal{R}_0$$

mass flux  ${m R}$ 

• cell movement (migration)



- cell growth (proliferation)
- cell division (hyperplasia)
- cell enlargement (hypertrophy)





### biological equilbrium

cowin & hegedus [1976], beaupré, orr & carter [1990], harrigan & hamilton [1992], jacobs, levenston, beaupré, simo & carter [1995], huiskes [2000], carter & beaupré [2001]

# growing bone as open system

#### problem 4 - wikipedia websites on growth

Create or edit a wikipedia website on growth. To create a site, you can think of any growth example. To edit a site, e.g., go to http://en.wikipedia.org/wiki/Wolff's\_law or http://en.wikipedia.org/wiki/Tissue\_expansion. Add at least one paragraph of text with at least two references. Ideally, even add a figure. Print your submission and hand it in with your homework.

#### problem 5 - revise your final project

#### homework #03

#### balance equations for open systems - momentum

• volume specific version

$$D_t(\rho_0 \boldsymbol{v}) = Div(\boldsymbol{P} + \boldsymbol{v} \otimes \boldsymbol{R}) + [\boldsymbol{b}_0 + \boldsymbol{v} \boldsymbol{\mathcal{R}}_0 - \nabla_X \boldsymbol{v} \cdot \boldsymbol{R}]$$

subraction of weighted balance of mass

$$\boldsymbol{v} \operatorname{D}_t \rho_0 = \operatorname{Div}(\boldsymbol{v} \otimes \boldsymbol{R}) + \boldsymbol{v} \mathcal{R}_0 - \nabla_X \boldsymbol{v} \cdot \boldsymbol{R}$$

mass specific version

$$\rho_0 \, \mathrm{D}_t \boldsymbol{v} = \mathrm{Div}(\boldsymbol{P}) + \boldsymbol{b}_0$$

### mechanical equilbrium

# growing bone as open system

### constitutive equations for open systems

• free energy  $\psi_0 = \left[\frac{\rho_0}{\rho_0^*}\right]^n \psi_0^{\mathrm{neo}}(F)$ 

• stress  $P = \left[\frac{\rho_0}{\rho_0^*}\right]^n P^{\mathrm{neo}}(F)$ 

• mass flux  $\boldsymbol{R} = R_0 \nabla_X \rho_0$ 

• mass source  $\mathcal{R}_0 = \left[\frac{\rho_0}{\rho_0^*}\right]^{-m} \psi_0(\mathbf{F}) - \psi_0^*$ 







### coupling of growth and deformation

gibson & ashby [1999]

### growing bone as open system

### staggered solution - integration point based



weinans, huiskes & grootenboer [1992], harrigan & hamilton [1992], [1994], jacobs, levenston, beaupré,simo & carter [1995]

### simultaneous solution - node point based



jacobs, levenston, beaupré, simo & carter [1995], fischer, jacobs, levenston & carter [1997], nackenhorst [1997], levenston [1997]]

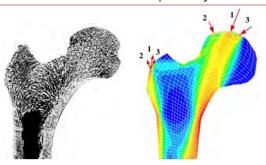
### sequential solution - element based



huiskes, weinans, grootenboer, dalstra, fudala & slooff [1987], carter, orr, fhyrie [1989], beaupré, orr & carter [1990], weinans, huiskes & grootenboer [1992], [1994], jacobs, levenston, beaupré, simo & carter [1995], huiskes [2000], carter & beaupré [2001]

# finite elements - integration point based 11

#### finite elements for open systems



- dense system of compressive trabaculae carrying stress into calcar region
- secondary arcuate system, medial joint surface to lateral metaphyseal region
- ward's triangle, low density region contrasting dense cortical shaft

carter & beaupré [2001]

### growing bone as open system



# recipe for finite element modeling

from continuous problem...

$$\begin{array}{rcl} \mathbf{D}_t \rho_0 &= \mathbf{Div}(\mathbf{\overset{\approx}{R}}) + \mathbf{\overset{\circ}{\mathcal{R}}_0} \\ \rho_0 \, \mathbf{D}_t \boldsymbol{v} &= \mathbf{Div}(\boldsymbol{P}) + \boldsymbol{b}_0 \end{array}$$

- temporal discretization implicit euler backward
- spatial discretization finite element method
- staggered/simultaneous newton raphson iteration
- linearization gateaux derivative

... to linearized discrete initial boundary value problem

finite elements - integration point based 12

### key transformation - from strong form to weak form (1d)

strong / differential form

$$\sum f = f^{\text{int}} + f^{\text{ext}} \doteq 0$$
  $f^{\text{int}} = P'(\varphi)$ 

strong form / residual format

$$\mathsf{R}(\varphi) = P'(\varphi) + f^{\mathrm{ext}} \doteq 0$$

 weak / integral form - nonsymmetric  $\forall \delta \varphi$ 

$$G(\delta \varphi; \varphi) = \int \delta \varphi \cdot [P'(\varphi) + f^{\text{ext}}] dx = 0$$

integration by parts

$$\int \delta \varphi \cdot P' dx = \int [\delta \varphi \cdot P]' dx - \int \delta \varphi' \cdot P dx$$

• integral theorem & neumann bc's

$$\int [\delta \varphi \cdot P]' dx = \delta \varphi \cdot P|_{x=0}^{x=l}$$

• weak form / integral form - symmetric  $\forall \delta \varphi$ 

$$\int \delta \varphi' \cdot P dx - \delta \varphi \cdot P|_{x=0}^{x=i} - \int \delta \varphi \cdot f^{\text{ext}} \doteq 0$$

### finite elements – integration point based 13

#### residual equation...

strong / differential form

$$\mathbf{R}^{\varphi} = \rho_0 \, \mathcal{D}_t v \, - \mathrm{Div}(\mathbf{P}) - b_0 = \mathbf{0} \, \text{in } \mathcal{B}_0$$

dirichlet / essential boundary conditions (displacements)

$$\varphi - \bar{\varphi} = \mathbf{0}$$
 on  $\partial \mathcal{B}_0^{\varphi}$  with  $\partial \mathcal{B}_0^{\varphi} \cup \partial \mathcal{B}_0^{T^{\varphi}} = \partial \mathcal{B}_0$ 

• neumann / natural boundary conditions (tractions)

$$P \cdot N - \bar{T}^{\varphi} = 0$$
 on  $\partial \mathcal{B}_0^{T^{\varphi}}$  and  $\partial \mathcal{B}_0^{\varphi} \cap \partial \mathcal{B}_0^{T^{\varphi}} = \emptyset$ 

finite elements – integration point based <sup>15</sup>

... and boundary conditions

# from equilibrium equation...

• start with nonlinear mechanical equilibrium equation



cast it into its residual format

$$\mathbf{R}^{\varphi}(\varphi) = \mathbf{0}$$
 in  $\mathcal{B}_0$ 

with residual

$$\mathbf{R}^{\varphi} = \rho_0 \, \mathbf{D}_t v \, - \mathrm{Div}(\mathbf{P}) - b_0$$

... to residual format

### finite elements – integration point based 14

### from strong form...

strong / differential form



in  $\mathcal{B}_0$ 

$$\mathbf{R}^{\varphi} = \rho_0 \, \mathcal{D}_t v \, - \mathrm{Div}(\mathbf{P}) - b_0 = \mathbf{0}$$

mulitplication with test function & integration

$$\mathsf{G}^{\varphi}\left(\delta\boldsymbol{\varphi};\boldsymbol{\varphi}\right) = \int_{\mathcal{B}_{0}} \delta\boldsymbol{\varphi} \cdot \mathbf{R}^{\varphi} dV = 0 \qquad \forall \delta\boldsymbol{\varphi} \text{ in } \mathcal{H}_{1}^{0}(\mathcal{B}_{0})$$

• weak form / nonsymmetric derivative derivative

$$\mathbf{G}^{\varphi} = \int_{\mathcal{B}_0} \delta \varphi \cdot \rho_0 \, \mathbf{D}_t v \, \mathrm{d}V - \int_{\mathcal{B}_0} \delta \overset{\bullet}{\varphi} \cdot \mathrm{Div}(\overset{\bullet}{P}) \mathrm{d}V - \int_{\mathcal{B}_0} \delta \varphi \cdot b_0 \, \mathrm{d}V$$

... to nonsymmetric weak form

### from non-symmetric weak form...

integration by parts



$$\int_{\mathcal{B}_0} \delta \boldsymbol{\varphi} \cdot \operatorname{Div}(\boldsymbol{P}) dV = \int_{\mathcal{B}_0} \operatorname{Div}(\delta \boldsymbol{\varphi} \cdot \boldsymbol{P}) dV - \int_{\mathcal{B}_0} \nabla \delta \boldsymbol{\varphi} : \boldsymbol{P} dV$$

- gauss theorem & boundary conditions  $\int_{\mathcal{B}_0} \operatorname{Div}(\delta \boldsymbol{\varphi} \cdot \boldsymbol{P}) dV = \int_{\partial \mathcal{B}_0^{T\varphi}} \boldsymbol{\varphi} \cdot \boldsymbol{P} \cdot \mathbf{N} dA = \int_{\partial \mathcal{B}_0^{T\varphi}} \delta \boldsymbol{\varphi} \cdot \bar{\boldsymbol{T}}^{\varphi} dA$
- weak form / symmetric first derivative derivative derivative

$$\mathsf{G}^{\varphi} = \int_{\mathcal{B}_0} \delta \varphi \cdot \rho_0 \, \, \mathsf{D}_t v \, \mathrm{d}V + \int_{\mathcal{B}_0} \nabla^{\mathsf{k}} \delta \varphi : \mathbf{P}^{\mathsf{k}} \mathrm{d}V - \int_{\partial \mathcal{B}_0^{T^{\varphi}}} \delta \varphi \, \bar{\mathbf{T}}^{\varphi} \mathrm{d}A - \int_{\mathcal{B}_0} \delta \varphi \, \cdot \, \mathbf{b}_0 \mathrm{d}V$$

... to symmetric weak form

### finite elements – integration point based <sup>17</sup>

#### from discrete weak form...

• discrete weak form



$$\mathsf{G}^{\varphi} = \delta \varphi_J \cdot \mathsf{R}_j^{\varphi}(\varphi_{n+1}^h) = 0$$

 $\forall \delta \boldsymbol{\varphi}_J$ 

• discrete residual format

$$\mathbf{R}^{\varphi}_{_{I}}(\boldsymbol{\varphi}_{n+1}^{h})=\mathbf{0}$$

$$\forall J=1,...,n_{\rm np}$$

discrete residual

$$\begin{aligned} \mathbf{R}_{J}^{\varphi} &= \mathbf{A}_{e=1}^{n_{\mathrm{el}}} \int_{\mathbb{S}_{0}^{e}} N_{\varphi}^{j} \mathbb{D}_{l} v_{n+1} \mathrm{d}V + \int_{\mathcal{B}_{0}^{e}} \nabla N_{\varphi}^{j} \cdot \mathbf{P}_{n+1} \mathrm{d}V \\ &- \int_{\partial \mathcal{B}_{0}^{e}} N_{\varphi}^{j} \, \bar{\mathbf{T}}_{n+1}^{\varphi} \mathrm{d}A - \int_{\mathbb{S}_{0}^{e}} N_{\varphi}^{j} b_{0\,n+1} \mathrm{d}V \end{aligned}$$

... to discrete residual

# spatial discretization

discretization

$$\mathcal{B}_0 = \bigcup_{e=1}^{n_{
m el}} \mathcal{B}_0^e$$



• interpolation of test functions

$$\delta \boldsymbol{\varphi}^h|_{\mathcal{B}_0^e} = \sum_{j=1}^{n_{\mathrm{en}}} N_{\varphi}^j \delta \boldsymbol{\varphi}_j \in \mathcal{H}_1^0(\mathcal{B}_0) \quad \nabla \delta \boldsymbol{\varphi}^h|_{\mathcal{B}_0^e} = \sum_{j=1}^{n_{\mathrm{en}}} \delta \boldsymbol{\varphi}_j \otimes \nabla N_{\varphi}^j$$

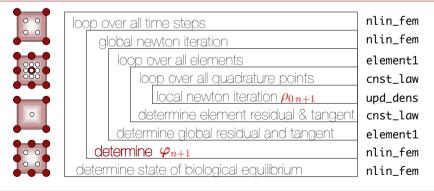
• interpolation of trial functions

$$|\varphi^h|_{\mathcal{B}_0^e} = \sum_{l=1}^{n_{\mathrm{en}}} N_{\varphi}^l \varphi_l \in \mathcal{H}_1(\mathcal{B}_0) \qquad \nabla \varphi^h|_{\mathcal{B}_0^e} = \sum_{l=1}^{n_{\mathrm{en}}} \varphi_l \otimes \nabla N_{\varphi}^l$$

... to discrete weak form

### finite elements - integration point based 18

### integration point based solution of balance of mass



staggered solution of density and displacements

finite elements - integration point based

#### nlin fem.m

```
for is = (nsteps+1):(nsteps+inpstep);
 iter = 0: residuum = 1:
while residuum > tol
   iter=iter+1;
   R = zeros(ndof,1); K = sparse(ndof,ndof);
   e_spa = extr_dof(edof,dof);
for ie = 1:nel
    [Ke,Re,Ie] = element1(e_mat(ie,:),e_spa(ie,:),i_var(ie,:),mat);
    [K, R, I] = assm_sys(edof(ie,:),K,Ke,R,Re,I,Ie);
u_inc(:,2)=dt*u_pre(:,2); R = R - time*F_pre;
   [dof,F] = solve_nr(K,R,dof,iter,u_inc);
   residuum= res_norm((dof-dofold),u_inc);
time = time + dt; i_var = I; plot_int(e_spa,i_var,nel,is);
```

### finite elements - integration point based 21

#### from discrete residual ...

linearization / newton raphson scheme

$$\mathbf{R}_{Jn+1}^{\varphi k+1} = \mathbf{R}_{Jn+1}^{\varphi k} + \mathrm{d}\mathbf{R}_{J}^{\varphi} \doteq 0 \quad \forall \ J = 1, ..., n_{\mathrm{np}}$$



incremental residual

$$\mathrm{d}\mathbf{R}_{J}^{\,arphi} = \sum_{L=1}^{n_{\mathrm{en}}} \mathbf{K}_{JL}^{arphi arphi} \cdot \mathrm{d}oldsymbol{arphi}_{L} \qquad \qquad \mathbf{K}_{JL}^{arphi arphi} = rac{\mathrm{d}\mathbf{R}_{J}^{arphi}}{\mathrm{d}oldsymbol{arphi}_{L}}$$

system of equations

$$\mathsf{K}_{JL}^{\varphi\varphi}\,\mathrm{d}arphi_L = -\mathsf{R}_{J\,n+1}^{\varphi\,k}$$

incremental iterative update

$$\Delta \varphi_L = \Delta \varphi_L + \mathrm{d} \varphi_L$$

$$\forall L = 1, ..., n_{\rm np}$$

... to linearized residual

# finite elements - integration point based 23

### integration point based



discrete residual

#### check in matlab!

$$\mathbf{R}_{J}^{\varphi} = \mathbf{A}_{e=1}^{n_{\mathrm{el}}} \int_{\mathcal{B}_{o}^{e}} \nabla N_{\varphi}^{j} \cdot \boldsymbol{P}_{n+1} \mathrm{d}V$$

residual of mechanical equilibrium/balance of momentum

righthand side vector for global system of equations

### finite elements - integration point based 22

#### linearized residual



stiffness matrix / iteration matrix

$$\mathbf{K}_{JL}^{\varphi\varphi} = \frac{\partial \mathbf{R}_{J}^{\varphi}}{\partial \varphi_{L}} = \mathbf{A}_{e=1}^{n_{\mathrm{el}}} \int_{\mathcal{B}_{0}^{e}} N_{\varphi}^{j} \rho \mathcal{D}_{\varphi}(\mathcal{D}_{t}v) N_{\varphi}^{l} \mathrm{d}V + \int_{\mathcal{B}_{0}^{e}} \nabla N_{\varphi}^{j} \cdot \mathbf{D}_{F} \mathbf{P} \cdot \nabla N_{\varphi}^{l} \mathrm{d}V$$

4th order tensor - derivatives of 2nd order tensors wrt 2nd order tensor

linearization of residual wrt nodal dofs.

iteration matrix for global system of equations

#### linearized residual



stiffness matrix / iteration matrix

#### check in matlab!

$$\mathbf{K}_{JL}^{\varphi\varphi} = \frac{\partial \mathbf{R}_{J}^{\varphi}}{\partial \boldsymbol{\varphi}_{L}} = \mathbf{A}_{e=1}^{n_{\mathrm{el}}} \int_{\mathcal{B}_{0}^{e}} \nabla N_{\varphi}^{j} \cdot \mathbf{D}_{F} \boldsymbol{P} \cdot \nabla N_{\varphi}^{l} \mathrm{d}V$$

linearization of residual wrt nodal dofs

iteration matrix for global system of equations

### finite elements - integration point based 25

#### quads 2d.m

```
for ip=1:4
indx=[2*ip-1; 2*ip]; detJ=det(JT(indx,:));
if detJ<10*eps; disp('Jacobi determinant less than zero!'); end;
JTinv=inv(JT(indx,:)); dNx=JTinv*dNr(indx,:);
F=zeros(2,2);
for i=1:4
  jndx=[2*j-1; 2*j];
  F=F+e\_spa(jndx)'*dNx(:,j)';
var = i_var(ip);
[A,P,var]=cnst_law(F,var,mat);
Ie(ip) = var;
for i=1:nod
  en=(i-1)*2:
           Re(en+ 1) +(P(1,1)*dNx(1,i)' ...
                  +P(1,2)*dNx(2,i)')*detJ*wp(ip);
  Re(en+ 2) = Re(en+ 2) + (P(2,1)*dNx(1,i)' ...
                  + P(2,2)*dNx(2,i)') * detJ * wp(ip);
%%% element stiffness matrix Ke, residual Re, internal variables Ie %%%
```

### finite elements - integration point based 27

#### quads 2d.m

```
function [Ke,Re,Ie]=element1(e_mat,e_spa,i_var,mat)
%%% element stiffness matrix Ke, residual Re, internal variables Ie %%%%
Re = zeros(8,1);
Ke = zeros(8,8);
nod=4:
             delta = eye(2);
indx=[1;3;5;7];
            ex_mat=e_mat(indx);
indy=[2;4;6;8]; ey_mat=e_mat(indy);
q1=0.577350269189626; w1=1;
ap(:,1)=[-g1; g1;-g1; g1];
                      w(:,1)=[ w1; w1; w1; w1];
gp(:,2)=[-g1;-g1; g1; g1];
                      w(:,2)=[ w1; w1; w1; w1];
wp=w(:,1).*w(:,2);
                  xsi=gp(:,1);
                                 eta=qp(:,2);
N(:,1)=(1-xsi).*(1-eta)/4;
                      N(:,2)=(1+xsi).*(1-eta)/4;
N(:,3)=(1+xsi).*(1+eta)/4;
                      N(:,4)=(1-xsi).*(1+eta)/4;
                      dNr(1:2:8, 2) = (1-eta)/4;
dNr(1:2:8,1)=-(1-eta)/4;
dNr(1:2:8,3) = (1+eta)/4;
                      dNr(1:2:8,4)=-(1+eta)/4;
dNr(2:2:8+1,1)=-(1-xsi)/4;
                      dNr(2:2:8+1,2)=-(1+xsi)/4;
dNr(2:2:8+1,3) = (1+xsi)/4;
                      dNr(2:2:8+1,4) = (1-xsi)/4;
JT=dNr*[ex_mat;ey_mat]';
%%% element stiffness matrix Ke, residual Re, internal variables Ie %%%%
```

# finite elements - integration point based 26

#### assm\_sys.m

```
function [K,R,I]=assm_sys(edof,K,Ke,R,Re,I,Ie)
%%% assemble local element contributions to global tangent & residual %
%%% input: edof = [ elem X1 Y1 X2 Y2 ]
                       ... incidence matrix
%%%
         = [ nedof x nedof ]
                        ... element tangent Ke
%%%
         = [fx_1 fy_1 fx_2 fy_2] \dots element residual Re
%%% output: K
         = [ ndof x ndof ]
                        ... global tangent K
         = [ ndof x 1 ]
                        ... global residual R
[nie,n]=size(edof);
I(edof(:,1),:)=Ie(:);
t=edof(:,2:n);
for i = 1:nie
 K(t(i,:),t(i,:)) = K(t(i,:),t(i,:))+Ke;
 R(t(i,:))
           =R(t(i,:))
```

#### @ integration point level

ullet constitutive equations - given  $oldsymbol{F} = 
abla oldsymbol{arphi}$  calculate  $oldsymbol{P}$ 



- update density for current stress state from  $\rho_{0n}$  and  $D_t \rho_0 = \left[\frac{\rho_0}{\rho_0^*}\right]^{-m} \psi_0(\mathbf{F}) - \psi_0^*$  calculate  $\rho_{0n+1}$
- calculate first piola kirchhoff stress of solid material

$$\boldsymbol{P}^{\text{neo}}(\boldsymbol{F}) = \mu_0 \, \boldsymbol{F} + [\lambda_0 \ln(\det(\boldsymbol{F})) - \mu_0] \boldsymbol{F}^{\text{-t}}$$

 calculate first piola kirchhoff stress of porous material  $P(F) = \left[\frac{\rho_0}{\rho_0^*}\right]^n P^{\text{neo}}$ 

stress for righthand side vector

finite elements - integration point based 29

#### @ integration point level

ullet constitutive equations - given F calculate  ${
m D}_F P$ 



$$\mathbf{D}_{F} \mathbf{P} = \partial_{F} \mathbf{P} - \partial_{\rho_{0}} \mathbf{P} \left[ \partial_{\rho_{0}} \mathcal{R}_{0} \right]^{1-} \partial_{F} \mathcal{R}_{0}$$

with

$$\begin{array}{ll} \partial_F \, \boldsymbol{P} &= \left[\frac{\rho_0}{\rho_0^*}\right]^n \left[\, \mu \boldsymbol{I} \overline{\otimes} \boldsymbol{I} + \lambda \boldsymbol{F}^{-t} \otimes \boldsymbol{F}^{-t} - \left[\lambda \ln J - \mu\right] \boldsymbol{F}^{-t} \underline{\otimes} \boldsymbol{F}^{-1} \,\right] \\ \partial_{\rho_0} \boldsymbol{P} &= \frac{1}{\rho_0} \, n \, \boldsymbol{P} \\ \partial_{\rho_0} \mathcal{R}_0 &= \left[\frac{\rho_0}{\rho_0^*}\right]^{-m} \frac{1}{\rho_0} \left[n - m\right] \psi_0 \end{array} \qquad \text{depending on time discretization}$$

$$\partial_F \, \mathcal{R}_0 = \left[ rac{
ho_0}{
ho_0^*} 
ight]^{-m} oldsymbol{P}$$

tangent for iteration matrix

### @ integration point level



ullet constitutive equations - given  $oldsymbol{F}$  calculate  $oldsymbol{P}$ 

check in matlab!

$$\mathbf{P}(\mathbf{F}) = \left[\frac{\rho_0}{\rho_0^*}\right]^n \mu_0 \mathbf{F} + \left[\lambda_0 \ln(\det(\mathbf{F})) - \mu_0\right] \mathbf{F}^{-t}$$

stress calculation @ integration point level

stress for righthand side vector

finite elements - integration point based <sup>30</sup>

#### @ integration point level



• tangent operator / constitutive moduli

check in matlab!

$$\mathbf{A} = D_F \mathbf{P} = \partial_F \mathbf{P} - \partial_{\rho_0} \mathbf{P} \left[ \partial_{\rho_0} \mathcal{R}_0 \right]^{1-} \partial_F \mathcal{R}_0$$

• linearization of stress wrt deformation gradient

tangent for iteration matrix

#### cnst den.m

```
function [A,P,var]=cnst_den(F,var,mat)
emod = mat(1); nue = mat(2); rho0 = mat(3); psi0 = mat(4);
expm = mat(5); expn = mat(6); dt = mat(7);
xmu = emod/2.0/(1.0+nue); xlm = emod * nue /(1.0+nue)/(1.0-2.0*nue);
F_{inv} = inv(F); J = det(F); delta = [1 0; 0 1];
Fvar.facs.factl=upd dens(F.var.mat):
P = facs * (xmu * F + (xlm * log(J) - xmu) * F_inv');
for i=1:2
for j=1:2
for k=1:2
for l=1:2
             * F_inv(j,i)*F_inv(l,k) ...
  A(i,j,k,l) = xlm
       - (xlm * log(J) - xmu) * F_inv(l,i)*F_inv(j,k) ...
         xmu * delta(i,k)*delta(j,l);
  A(i,j,k,l) = facs * A(i,j,k,l) + fact * P(i,j)*P(k,l);
end, end, end, end
```

### finite elements - integration point based



### recipe for temporal discretization

implicit euler backward

evolution of density

$$\mathrm{D}_t 
ho_0 = rac{1}{\Delta t} [
ho_{0\,n+1} - 
ho_{0\,n}]$$
 finite difference approximation

 $\mathbf{D}_t \rho_0 = \left[\frac{\rho_0}{\rho_0^*}\right]^{-m} \psi_0(\boldsymbol{F}) - \psi_0^*$ • discrete residual

$$\mathsf{R}_{n+1}^{\rho} = \frac{1}{\Delta t} [\rho_{0\,n+1} - \rho_{0\,n}] - \left[\frac{\rho_{0\,n+1}}{\rho_{\bullet}^*}\right]^{-m} \psi_0(\mathbf{F}) - \psi_0^* \doteq 0$$

euler backward

• local newton iteration

$$\begin{aligned} \mathsf{R}^{\rho k+1}_{n+1} &= \mathsf{R}^{\rho k}_{n+1} + \mathrm{d}\mathsf{R}^{\rho} \doteq 0 \\ \rho_{0\,n+1} &\leftarrow \rho_{0\,n+1} + \mathrm{d}\rho_0 \quad \mathrm{d}\rho_0 = \left[\frac{\mathrm{d}\mathsf{R}^{\rho}}{\mathrm{d}\rho_0}\right]^{-1} \mathsf{R}^{\rho k}_{n+1} \quad \text{iterative update} \end{aligned}$$

unconditionally stable - larger time steps

finite elements - integration point based 35



## recipe for temporal discretization

### explicit euler forward

evolution of density

$$\mathrm{D}_t 
ho_0 = rac{1}{\Delta t} [
ho_{0\,n+1} - 
ho_{0\,n}]$$
 finite difference approximation  $\mathrm{D}_t 
ho_0 = \left[rac{
ho_0}{
ho_0^*}
ight]^{-m} \psi_0(F) - \psi_0^*$  euler forward

direct update of growth multiplier

$$\rho_{0\,n+1} = \rho_{0\,n} + \left[ \left[ \frac{\rho_{0\,n}}{\rho_0^*} \right]^{-m} \psi_0\left(\boldsymbol{F}\right) - \psi_0^* \right] \Delta t$$

conditionally stable - limited time step size

### finite elements - integration point based 34

### @ integration point level



• discrete residual of density update

check in matlab!

$$\mathsf{R}_{n+1}^{\rho} = \frac{1}{\Delta t} [\rho_{0\,n+1} - \rho_{0\,n}] - \left[\frac{\rho_{0\,n+1}}{\rho_0^*}\right]^{-m} \psi_0(\mathbf{F}) - \psi_0^* \doteq 0$$

residual of biological equilibrium / balance of mass

local newton iteration

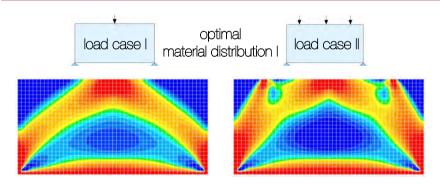
finite elements - integration point based 36

#### upd dens.m

```
function [var,facs,fact]=upd_dens(F,var,mat)
tol = 1e-8:
          var = 0.0;
xmu = emod / 2.0 / (1.0+nue);
                    xlm = emod * nue /(1.0+nue)/(1.0-2.0*nue);
J = det(F); C = F'*F;
                    I1 = trace(C);
psi0_neo = xlm/2 * log(J)^2 + xmu/2 * (I1 - 2 - 2*log(J));
              rho_k1 = (1+var)*rho0;
rho k0 = (1+var)*rho0:
                               iter = 0:
                                       res = 1:
while abs(res) > tol
 iter=iter+1;
 res =((rho_k1/rho0)^(expn-expm)*psi0_neo-psi0)*dt-rho_k1+rho_k0;
 dres= (expn-expm)*(rho_k1/rho0)^(expn-expm)*psi0_neo*dt/rho_k1-1;
 drho=- res/dres;     rho_k1 = rho_k1+drho;
rho = rho k1: var = rho / rho0 - 1:
facs = (rho/rho0)^expn;
facr = 1/dt - (expn-expm) * (rho/rho0)^(expn-expm) / rho *psi0_neo;
         expn / rho * (rho/rho0)^( -expm) / facr;
```

### finite elements - integration point based

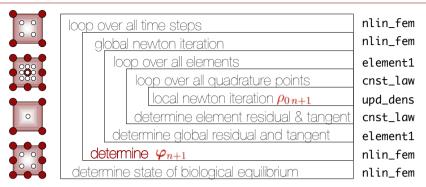
#### form follows function - bioinspired design



find the lightest structure to support a given set of loads

example - topology optimization

### integration point based solution of balance of mass



staggered solution of density and displacements

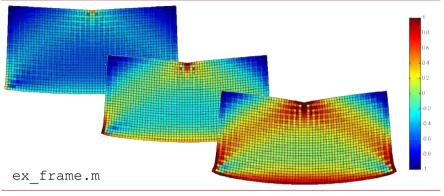
### finite elements - integration point based

#### ex frame.m

```
% function [q0,edof,bc,F_ext,mat,nel,node,ndof,nip] = ex_frame
emod = 1000; nue = 0.3; rho0 = 1.0; psi0 = 1.0;
expm = 3.0; expn = 2.0; dt = 1.0;
mat = [emod, nue, rho0, psi0, expm.expn.dt];
xbox(1) = 0.0; xbox(2) = 2.0; nx = 8;
ybox(1) = 0.0; ybox(2) = 1.0; ny = 4;
[q0,edof] = mesh_sqr(xbox,ybox,nx,ny);
[nel, sizen] = size(edof);[ndof,sizen] = size(q0);
         = ndof/2;
                     nip = 4;
%%% dirichlet boundary conditions
bc(1.1) = 2*(nv+1)*(0)
                             bc(1,2) = 0;
                     ) +2;
bc(2,1) = 2*(ny+1)*(nx
                     ) +2;
                             bc(2,2) = 0;
bc(3,1) = 2*(ny+1)*(nx/2+0) +1;
                             bc(3,2) = 0;
bc(4,1) = 2*(ny+1)*(nx/2+1)
                            bc(4,2) = -ybox(2)/50;
%%% neumann boundary conditions
F_{ext} = zeros(ndof,1);
%%% input data for frame example
```

### example - topology optimization

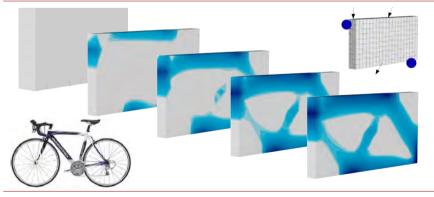
### form follows function - bioinspired design



find the lightest structure to support a given set of loads

# example - topology optimization

### form follows function



design of bicycle frame

example - topology optimization

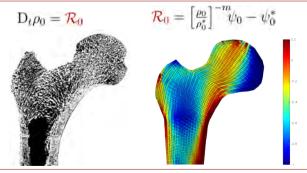
### form follows function



bicycle frames 1817-2005

# example - topology optimization

### functional adaptation of proxima femur



the density develops such that the tissue can just support the given mechanical load

# example - growing bone



#### femoral neck deformity

the femoral neck normally forms an angle of 120-135 degrees with the shaft of the bone. this acts

as the lever in easing the action of the muscles around the hip joint. an increase or decrease in this angle beyond the normal limits causes improper action of muscles, and interferes with walking. an increase in the angle beyond 135 degrees is called **coxa valga** or outward curvature of the hip joint. a decrease in the angle below 120 degrees is called **coxa vara** or inward curvature of the hip joint.

# example - femoral neck deformity

45

560

Computational modeling of bone density profiles in response to gait: A subject-specific approach

Henry Pang<sup>1</sup>, Abhishek P. Shiwalkar<sup>1</sup>, Chris M. Madormo<sup>1</sup>, Rebecca E. Taylor<sup>1</sup>, Thomas P. Andriacchi<sup>1,2</sup>, Ellen Kuht<sup>1,3,4</sup>





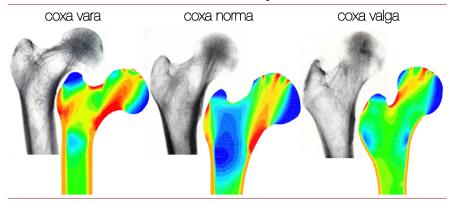
94.9

94.4

pang, shiwalkar, madormo, taylor, andriacchi, kuhl [2012]

example - henry's knee

#### simulation vs. x-ray scans

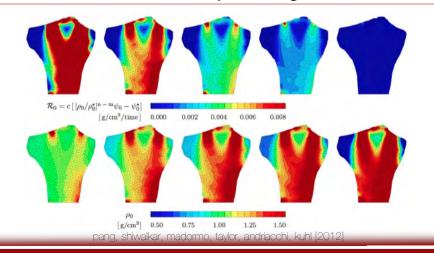


excellent agreement of simulation and x-ray pattern

pauwels [1973], balle [2004], kuhl & balle [2005]

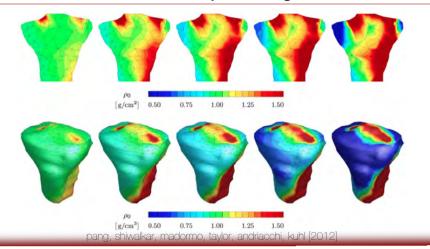
### example - femoral neck deformity

### how does henry's bone grow?



example - henry's knee

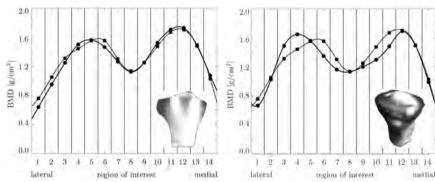
### how does henry's bone grow?



# example - henry's knee

# how predictive is the simulation?





pang, shiwalkar, madormo, taylor, andriacchi, kuhl [2012]

example - henry's knee

# how predictive is the simulation?

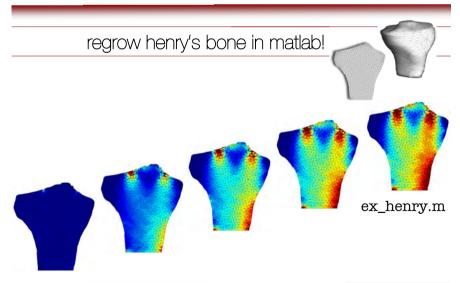




|                    | DEXA<br>[g/cm <sup>2</sup> ] | $2d$ FEM $[g/cm^2]$ | 2d error<br>[%] | 3d FEM<br>[g/cm <sup>3</sup> ] | 3d error<br>[%] |
|--------------------|------------------------------|---------------------|-----------------|--------------------------------|-----------------|
| BMD <sub>lat</sub> | 1.268                        | 1.233               | 2.73            | 1.384                          | 9.33            |
| BMD <sub>med</sub> | 1.621                        | 1.637               | 0.99            | -1.556                         | 3.99            |
|                    | DEXA                         | 2d FEM              | 2d error<br>[%] | 3d FEM                         | 3d error<br>[%] |
| M:L-ratio          | 1.279                        | 1.327               | 3.83            | 1.122                          | 12.18           |

pang, shiwalkar, madormo, taylor, andriacchi, kuhl [2012]

# example - henry's knee



pang, shiwalkar, madormo, taylor, andriacchi, kuhl [2012]

example - henry's knee