

# A nonlinear coupling of chemical kinetics with mechanics

V. Klika<sup>1,2</sup>, M. Grmela<sup>3</sup>

<sup>1</sup>Institute of Thermomechanics of the AS CR, CR  
klika@it.cas.cz

<sup>2</sup>Dept. of Mathematics, FNSPE, Czech Technical University in Prague, CR

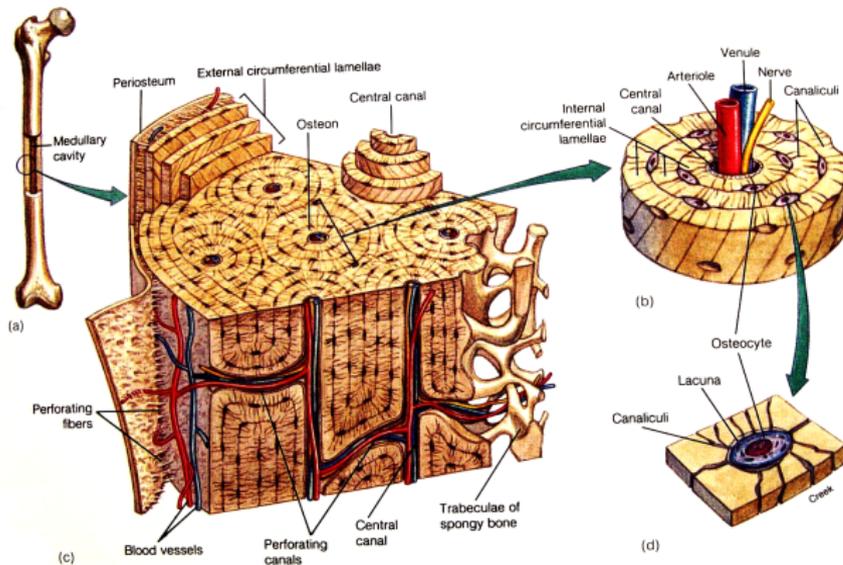
<sup>3</sup>Chemical Engineering, Ecole Polytechnique, Montreal, Canada

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# Outline

- 1 Motivation
- 2 A first approximation of coupling - CIT
- 3 A non-linear mechano-chemical coupling - GENERIC
- 4 A feedback to motivation?
- 5 Conclusions

# Bone and BR



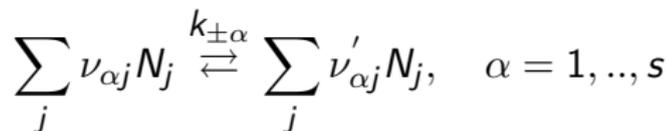
Why are we interested?

- the importance of mechanics (coupling)
- two groups of models (lack of communication)
- bridging them with NET

Functions of BR in bone: to keep bone alive, to alter the shape of bone, repair damages in bone tissue, part of metabolism

## Finding model formulation I

- For interaction schemes



the *Law of Mass Action* is used (with some limitations)

$$r_\alpha = k_{+\alpha} \prod_{j=1}^n [N_j]^{\nu_{\alpha j}} - k_{-\alpha} \prod_{j=1}^n [N_j]^{\nu'_{\alpha j}}$$

- Consequently, the change in concentration of subst. in time

$$[\dot{N}_j] = \sum_{\alpha} (\nu_{\alpha j} - \nu'_{\alpha j}) r_{\alpha}$$

where  $j$  refers to a substance  $N_j$ ,  $r_{\alpha}$  is the rate of  $\alpha$ -th interaction,  $\nu_{\alpha j}$  is stoichiometric coefficient for entering, outcoming substances  $N_j$  of interaction  $\alpha$ , respectively

# Finding model formulation of II

## Phenomenological relations

### Entropy production

$$\sigma(S) = \mathbf{j}_q \nabla \frac{1}{T} - \sum_{i=1}^n \mathbf{j}_{Di} \left( \nabla \frac{\mu_i}{T} - \frac{\mathbf{F}_i}{T} \right) + \frac{1}{T} \mathbf{t}_{\text{dis}} : \nabla \mathbf{v} + \frac{1}{T} \sum_{\alpha=1}^s r_\alpha \mathcal{A}_\alpha \geq 0.$$

and its general form:

$$\sigma(S) = J_S X_S + \mathbf{J}_V \cdot \mathbf{X}_V + \mathbf{J}_a^a \cdot \mathbf{X}_a^a + \mathbf{J}_t : \mathbf{X}_t.$$

CIT for a scalar (rate of chemical reaction):

$$J_S = L_{SS} X_S + \mathbf{L}_{SV} \cdot \mathbf{X}_V + \mathbf{L}_{Sa}^a \cdot \mathbf{X}_a^a + \mathbf{L}_{st(s)}^o : \mathbf{X}_{t(s)}^o.$$

WLOG  $\mathbf{L}_{st}$  is of the same kind as the thermodynamic force  $\mathbf{X}_t$  (thus,

$\mathbf{L}_{st}^o = \mathbf{L}_{st(s)}^o$  is a symmetric tensor with zero trace)

## Rate of deformation tensor and entropy production

$$\mathbf{D}^{ij} = \dot{\mathbf{E}}^{ij} = \frac{1}{2} \left( \frac{\partial \dot{\mathbf{u}}^i}{\partial x^j} + \frac{\partial \dot{\mathbf{u}}^j}{\partial x^i} \right) = \frac{1}{2} \left( \frac{\partial \mathbf{v}^i}{\partial x^j} + \frac{\partial \mathbf{v}^j}{\partial x^i} \right) = \frac{1}{2} ((\nabla \mathbf{v})^{ij} + (\nabla \mathbf{v})^{ji}),$$

and for the rate of volume variation  $\mathbf{D}^{(1)}$  it holds:

$$\mathbf{D}^{(1)} = \dot{\mathbf{E}}^{(1)} = \operatorname{div} \mathbf{v} = -\frac{1}{\rho} \frac{d\rho}{dt}$$

note: tensor  $\mathbf{D}$  is the symmetric part of tensor  $\nabla \mathbf{v}$  and thus

$$\begin{aligned} T\sigma(S) &= \mathbf{t}_{\text{dis}} : \nabla \mathbf{v} + \sum_{\alpha=1}^s r_{\alpha} \mathcal{A}_{\alpha} = \\ &= \left( \sum_{\alpha=1}^s r_{\alpha} \mathcal{A}_{\alpha} + \frac{1}{3} \operatorname{tr}(\nabla \mathbf{v}) \operatorname{tr}(\mathbf{t}_{\text{dis}}) \right) + (\nabla \mathbf{v})_{(a)} \cdot (\mathbf{t}_{\text{dis}})_{(a)} + \overset{\circ}{\mathbf{D}} : (\overset{\circ}{\mathbf{t}}_{\text{dis}})_{(s)} \geq 0, \end{aligned}$$

where  $\nabla \mathbf{v}$  was decomposed into scaled unit tensor and a symmetric and an antisymmetric parts with zero traces.

## The isotropic system

To recall:

$$J_s = L_{ss}X_s + \mathbf{L}_{sv} \cdot \mathbf{X}_v + \mathbf{L}_{sa}^a \cdot \mathbf{X}_a + \mathbf{L}_{st(s)}^{\circ} : \mathbf{X}_{t(s)}^{\circ}.$$

Constraints on phenomenological coefficients follow (from invariance of isotropic system under orthogonal transformations - does not modify the phenomenological tensors): inversion ( $\mathbf{L}_{sv} = 0$ ), arbitrary rotation ( $\mathbf{L}_{sa}^a = 0$ )

Finally, from the fact that scalar quantity is not affected by orthogonal transf, namely  $\mathbf{a}^T \mathbf{b}$  it follows

$$\mathbf{L}_{st} = L_{st} \mathbf{U}.$$

Moreover,  $\text{tr } \mathbf{L}_{st} = 0 \Rightarrow \mathbf{L}_{st} = 0.$

In total (Curie principle):

$$J_s = L_{ss}X_s$$

or in particular

$$r_\alpha = L_{s1}A_\alpha + L_{s2}D^{(1)}.$$

## Other choices of decomposition - scalar quantity $\mathbf{D}^{(2)}$

Analogous procedure; difference - tensors are not traceless

Still constraints on phenomenological coefficients follow (from invariance of isotropic system under orthogonal transformations - does not modify the phenomenological tensors): inversion ( $\mathbf{L}_{sv} = 0$ ), arbitrary rotation ( $\mathbf{L}_{sa}^a = 0$ ) but  $\mathbf{L}_{st} \neq 0$ , only

$$\mathbf{L}_{st} = L_{st} \mathbf{U},$$

In total, CIT and Curie-Prigogine principle leads to (notice the dynamic origin; static l. when viscous effects are significant but still through strain rate)

$$\begin{aligned} r_\alpha &= L_{s_1} \mathcal{A}_\alpha + \boxed{L_{s_2} \mathbf{D}^{(1)}} \\ &= L_{s_1} \mathcal{A}_\alpha + L_{s_2} \mathbf{D}^{(2)} + \boxed{L_{s_3} \mathbf{D}^{(1)}}. \end{aligned}$$

# Finding model formulation III

## Modified Law of Mass Action

The most important (least worst option) invariant is  $\mathbf{D}^{(1)}$  and thus

$$\implies r_\alpha = l_{\alpha\alpha}\mathcal{A}_\alpha + l_{\alpha\nu}\mathbf{D}^{(1)}$$

Expressions of affinity and chemical potential in CIT lead to

- 1 The Law of Mass Action (when coupling neglected)

$$r_\alpha = l_{\alpha\alpha}\mathcal{A}_\alpha = k_{+\alpha} \prod_{j=1}^n [\text{N}_j]^{\nu_{\alpha j}} - k_{-\alpha} \prod_{i=1}^n [\text{N}_i]^{\nu'_{\alpha i}}$$

- 2 The modified Law of Mass Action (including mechano-chemical coupling)

$$r_\alpha = l_{\alpha\alpha}\mathcal{A}_\alpha + l_{\alpha\nu}\mathbf{D}^{(1)} = k_{+\alpha} \prod_{j=1}^n [\text{N}_j]^{\nu_{\alpha j}} - k_{-\alpha} \prod_{i=1}^n [\text{N}_i]^{\nu'_{\alpha i}} + l_{\alpha\nu}\mathbf{D}^{(1)}$$

$$(C^{ijkl} = C^{ijkl}(\text{N}_j) = C^{ijkl}(\text{N}_j(\mathbf{D}^{(1)})))$$

# Prerequisites

- Isothermal -  $\phi$  instead of  $S$
- Mechanical *scalar* variables (coupling depends on parity): even-parity  $\mathbf{a}$ , and odd-parity  $\mathbf{b}$
- Chemical variables: molar concentrations  $\mathbf{n}$  and their fluxes  $\mathbf{z}$
- Conjugates  $(\mathbf{a}^*, \mathbf{b}^*)$ ,  $(\mathbf{n}^*, \mathbf{z}^*)$ ,  $\mathbf{a}^* = \partial_{\mathbf{a}}\phi$

## Uncoupled mechanics

The time evolution of simplified but complete mechanics relevant for coupling (GENERIC):

$$\begin{aligned} \begin{pmatrix} \dot{\mathbf{a}} \\ \dot{\mathbf{b}} \end{pmatrix} &= \begin{pmatrix} 0 & \boldsymbol{\kappa} \\ -\boldsymbol{\kappa}^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \end{pmatrix} - \begin{pmatrix} 0 \\ \Theta_{\mathbf{b}^*}^{mech} \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{\kappa} \mathbf{b}^* \\ -\boldsymbol{\kappa}^T \mathbf{a}^* \end{pmatrix} - \begin{pmatrix} 0 \\ \Theta_{\mathbf{b}^*}^{mech} \end{pmatrix}. \end{aligned}$$

The dissipation potential  $\Theta^{mech}(\mathbf{a}, \mathbf{b}^*)$  satisfies:

$\Theta^{mech}$  is a real valued and sufficiently regular function of  $(\mathbf{a}, \mathbf{b}, \mathbf{b}^*)$

$\Theta^{mech}(\mathbf{a}, \mathbf{b}, 0) = 0$

$\Theta^{mech}(\mathbf{a}, \mathbf{b}, \mathbf{b}^*)$  reaches its minimum at  $\mathbf{b}^* = 0$

$\Theta^{mech}(\mathbf{a}, \mathbf{b}, \mathbf{b}^*)$  is a convex function of  $\mathbf{b}^*$  in a neighbourhood of  $\mathbf{b}^* = 0$ .

$\Theta^{mech}$  is usually considered quadratic.

## Notes on structure of the evolution eq

$$\begin{aligned} \begin{pmatrix} \dot{\mathbf{a}} \\ \dot{\mathbf{b}} \end{pmatrix} &= \begin{pmatrix} 0 & \boldsymbol{\kappa} \\ -\boldsymbol{\kappa}^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \end{pmatrix} - \begin{pmatrix} 0 \\ \Theta_{\mathbf{b}^*}^{mech} \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{\kappa} \mathbf{b}^* \\ -\boldsymbol{\kappa}^T \mathbf{a}^* \end{pmatrix} - \begin{pmatrix} 0 \\ \Theta_{\mathbf{b}^*}^{mech} \end{pmatrix}, \end{aligned}$$

**The first term:** time reversibility (invariance under  $t \rightarrow -t$  and change of parity).

**The second term:** in mechanics, dissipation is typically a friction  $\propto$  lin momenta  $\mathbf{b} \Rightarrow$  dissipation term has odd-parity;  $\Rightarrow$  dissipation term is expected to be only in the evolution of linear momentum  $\mathbf{b}$ ; We let only the odd-parity variables dissipate

Note that  $\frac{d\Phi}{dt} \leq 0$  (consistency with thermodynamics).

# Uncoupled chemistry, LoMA

LoMA (Guldberg-Waage) in GENERIC form (yesterday):

$$\dot{\mathbf{n}} = -\Xi_{\mathbf{n}^*}^{chem}$$

with dissipation potential

$$\Xi^{chem}(\mathbf{n}, \mathbf{X}) = \sum_{\rho=1}^s W_{\rho}(\mathbf{n}) \left( e^{-\frac{1}{2}X_{\rho}} + e^{\frac{1}{2}X_{\rho}} - 2 \right)$$

where thermodynamic forces  $\mathbf{X} = (X_1, \dots, X_s)^T$  are

$$X_{\rho} = \sum_{k=1}^K \gamma_{\rho}^k \Phi_{n_k}^{chem}$$

together with the natural choice of entropy form  $S(\mathbf{n}) = -\sum_{j=1}^K (n_j \ln n_j + Q_j n_j)$  where  $Q_1, \dots, Q_K$  can be calculated.

Note that  $\mathbf{n}^* = \boldsymbol{\mu}$ .

## Uncoupled chemistry, Extended

Fluxes (odd-parity momentum-like quantity) considered as independent variables (motivated by EIT; yesterday)

From the analogy with mechanics

$$\begin{aligned} \begin{pmatrix} \dot{\mathbf{n}} \\ \dot{\mathbf{z}} \end{pmatrix} &= \begin{pmatrix} 0 & \gamma \\ -\gamma^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{n}^* \\ \mathbf{z}^* \end{pmatrix} - \begin{pmatrix} 0 \\ \Theta_{\mathbf{z}^*}^{chem} \end{pmatrix} \\ &= \begin{pmatrix} \gamma \mathbf{z}^* \\ -\gamma^T \mathbf{n}^* \end{pmatrix} - \begin{pmatrix} 0 \\ \Theta_{\mathbf{z}^*}^{chem} \end{pmatrix} \end{aligned}$$

Note that the reversible part of the right-hand-side of  $\dot{\mathbf{z}}$  is equal to affinity. The standard LoMA formulation in GENERIC is required when fluxes equilibrate (separation of timescales)  $\rightarrow$  dissipative potential  $\Theta^{chem}$ . Now  $\mathbf{n}$  acquire dissipation.

## Coupled chemical kinetics and mechanics

$$\begin{aligned}
 \begin{pmatrix} \dot{\mathbf{n}} \\ \dot{\mathbf{a}} \\ \dot{\mathbf{z}} \\ \dot{\mathbf{b}} \end{pmatrix} &= \begin{pmatrix} 0 & 0 & \gamma & \mu \\ 0 & 0 & \nu & \kappa \\ -\gamma^T & -\nu^T & 0 & 0 \\ -\mu^T & -\kappa^T & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{n}^* \\ \mathbf{a}^* \\ \mathbf{z}^* \\ \mathbf{b}^* \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ \Theta_{\mathbf{z}^*}^{(1,n,a,z,b)} \\ \Theta_{\mathbf{b}^*}^{(2,n,a,z,b)} \end{pmatrix} \\
 &= \begin{pmatrix} \gamma\mathbf{z}^* + \mu\mathbf{b}^* \\ \kappa\mathbf{b}^* + \nu\mathbf{z}^* \\ -\gamma^T\mathbf{n}^* - \nu^T\mathbf{a}^* - \Theta_{\mathbf{z}^*}^{(1,n,a,z,b)} \\ -\kappa^T\mathbf{a}^* - \mu^T\mathbf{n}^* - \Theta_{\mathbf{b}^*}^{(2,n,a,z,b)} \end{pmatrix}
 \end{aligned}$$

Again dissipation is assumed only in evolution of odd-parity variables and reversible evolution of a state variable is caused by conjugate state variables with different parity

## Coupling, separation of scales

Relaxation times of reaction fluxes  $\ll$  relaxation times of concentrations, i.e.  $\dot{\mathbf{z}} = 0$  with solution  $\mathbf{z}^* = \mathbf{Z}^*(\mathbf{n}, \mathbf{a}, \mathbf{b})$  (we aim for modified LoMA). The time evolution equations become now

$$\begin{pmatrix} \dot{\mathbf{n}} \\ \dot{\mathbf{a}} \\ \dot{\mathbf{b}} \end{pmatrix} = \begin{pmatrix} \gamma \mathbf{Z}^* + \mu \mathbf{b}^* \\ \kappa \mathbf{b}^* + \nu \mathbf{Z}^* \\ -\kappa^T \mathbf{a}^* - \mu^T \mathbf{n}^* - \Theta_{\mathbf{b}^*}^{(2,n,a,Z,b)} \end{pmatrix}.$$

Note the linear dependence of  $\dot{\mathbf{n}}$  on odd-parity conjugate variables  $\mathbf{b}^*$  (CIT, Casimir-Onsager).

## Further insight, a particular example I

State variables  $(\mathbf{n}, \mathbf{a}, \mathbf{b})$  and entropy of the form

$$S(\mathbf{n}, \mathbf{a}, \mathbf{b}) = - \sum n_j \ln n_j + Q_j n_j + \tilde{S}(\mathbf{a}, \mathbf{b}).$$

Assuming separation of dissipation potential

$$\Xi(\mathbf{n}, \mathbf{a}, \mathbf{b}, \mathbf{n}^*, \mathbf{a}^*, \mathbf{b}^*) = \Xi^1(\mathbf{n}, \mathbf{a}, \mathbf{b}, \mathbf{n}^*) + \Xi^2(\mathbf{n}, \mathbf{a}, \mathbf{b}, \mathbf{a}^*, \mathbf{b}^*).$$

Then the evolution is:

$$\begin{pmatrix} \dot{\mathbf{n}} \\ \dot{\mathbf{a}} \\ \dot{\mathbf{b}} \end{pmatrix} = \begin{pmatrix} \gamma \mathbf{Z}^* + \mu \mathbf{b}^* \\ \kappa \mathbf{b}^* + \nu \mathbf{Z}^* \\ -\kappa^T \mathbf{a}^* - \mu^T \mathbf{n}^* - \Xi_{\mathbf{b}^*}^2 \end{pmatrix},$$

where  $\mathbf{z}^* = \mathbf{Z}^*(\mathbf{n}, \mathbf{a}, \mathbf{b}, \mathbf{n}^*, \mathbf{a}^*)$  is the solution of zero flux equation

$$\gamma^T \mathbf{n}^* + \nu^T \mathbf{a}^* + \Xi_{\mathbf{z}^*} = 0 \text{ (quasi-steady assumption).}$$

## Further insight, a particular example II

Now, as  $\Xi_{z^*} = \Xi_{z^*}^1(z^*)$  we identify  $\Xi^1(z^*)$  with the dissipation potential for uncoupled chemical kinetics  $\Theta^{chem}(z^*)$ .

Then

$$\Xi_{z_\rho}^1 = \Theta_{z_\rho}^{chem} = -2 \ln \left( -\frac{z_\rho^*}{W_\rho} + \sqrt{\left(\frac{z_\rho^*}{W_\rho}\right)^2 + 1} \right) = - \underbrace{\left( \gamma^T \mathbf{n}^* + \nu^T \mathbf{a}^* \right)}_{X_\rho}$$

$$\therefore \mathbf{Z}_\rho^*(\mathbf{n}^*, \mathbf{a}^*) = -\frac{1}{2} W_\rho \left( e^{1/2 X_\rho} - e^{-1/2 X_\rho} \right)$$

$$\therefore -(\gamma \mathbf{Z}^*(\mathbf{n}^*, \mathbf{a}^*))_k = - \sum_\rho \gamma_\rho^k \mathbf{Z}_\rho^*(\mathbf{n}^*, \mathbf{a}^*)$$

which is exactly the chemical dissipation potential  $\Theta_{\mathbf{n}^*}^{chem}$  yielding the law of mass action within GENERIC but where “extended affinities”

$$X_\rho = \left( \gamma^T \mathbf{n}^* + \nu^T \mathbf{a}^* \right)_\rho$$

have been introduced.

Note that  $X_\rho$  is independent of  $\mathbf{b}^*$ . LoMA is recovered without coupling,  $\nu = 0$ ,  $\mu = 0$ .

## Further insight, a particular example III

The evolution equations may now be rewritten into the following form

$$\begin{pmatrix} \dot{\mathbf{n}} \\ \dot{\mathbf{a}} \\ \dot{\mathbf{b}} \end{pmatrix} = \begin{pmatrix} 0 & 0 & \boldsymbol{\mu} \\ 0 & 0 & \boldsymbol{\kappa} \\ -\boldsymbol{\mu}^T & -\boldsymbol{\kappa}^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{n}^* \\ \mathbf{a}^* \\ \mathbf{b}^* \end{pmatrix} - \begin{pmatrix} \Xi_{\mathbf{n}^*}^1 \\ \Xi_{\mathbf{a}^*}^1 \\ \Xi_{\mathbf{b}^*}^2 \end{pmatrix},$$

where

$$\Xi^1(\mathbf{n}, \mathbf{a}, \mathbf{b}, \mathbf{n}^*, \mathbf{a}^*) = \sum_{\rho=1}^s W_{\rho}(\mathbf{n}) \left( e^{-\frac{1}{2}X_{\rho}} + e^{\frac{1}{2}X_{\rho}} - 2 \right)$$

with  $X_{\rho} = \sum_j \gamma_{\rho}^j n_j^* + \sum_i \nu_{\rho}^i a_i^*$  and  $\Xi^2(\mathbf{n}, \mathbf{a}, \mathbf{b}, \mathbf{a}^*, \mathbf{b}^*)$  being some relevant dissipation functional for description of the considered mechanical process (standard potential would be quadratic).

## Further insight, a particular example IV

### Modified LoMA

The very same calculations that lead to obtaining the law of mass action within GENERIC may be applied here yielding

$$\dot{n}_i = \underbrace{\sum_{\rho} \left\{ \vec{k}_{\rho} \exp \left( -\frac{1}{2} \sum_j \nu_{\rho}^j a_{\rho}^* \right) \right\}}_{\vec{k}_{\rho}} \gamma_{\rho}^i \prod_l n_l^{\alpha_{\rho}^l} - \underbrace{\sum_{\rho} \left\{ \overleftarrow{k}_{\rho} \exp \left( \frac{1}{2} \sum_j \nu_{\rho}^j a_j^* \right) \right\}}_{\overleftarrow{k}_{\rho}} \gamma_{\rho}^i \prod_l n_l^{\beta_{\rho}^l} + \sum_j \mu_j^i b_j^*, \quad i = 1, \dots, K$$

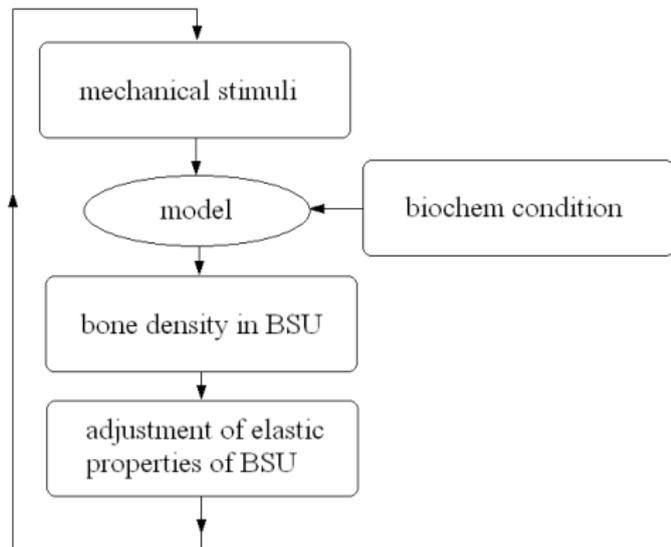
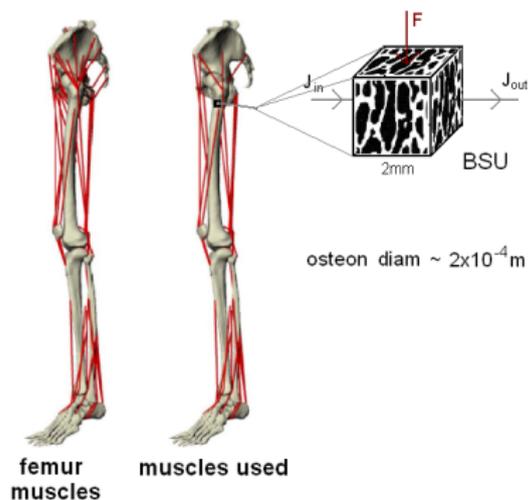
and for mechanics

$$\dot{a}_i = \sum_{\rho} \vec{k}_{\rho} \nu_{\rho}^i \prod_l n_l^{\alpha_{\rho}^l} - \sum_j \overleftarrow{k}_{\rho} \nu_{\rho}^j \prod_l n_l^{\beta_{\rho}^l} + \sum_j \kappa_j^i b_j^*, \quad i = 1, \dots, m_1$$

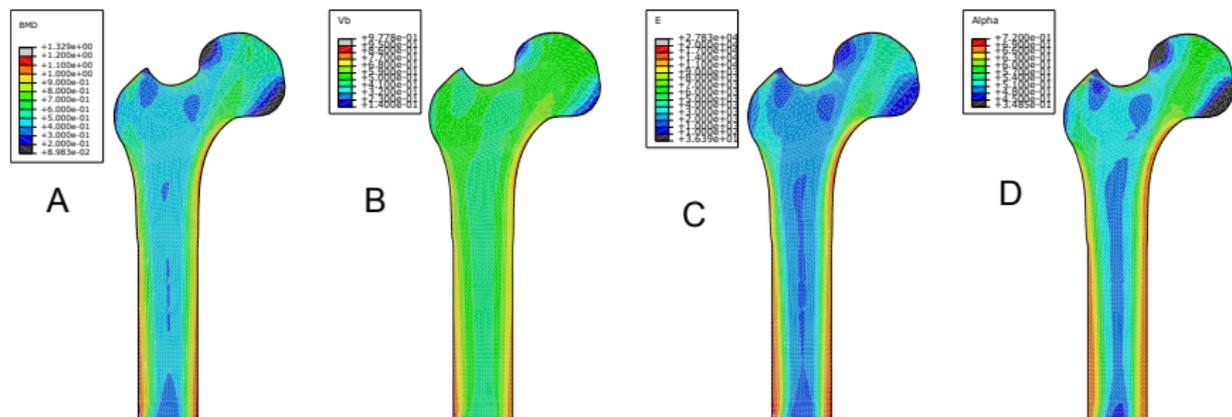
$$\dot{b}_i = - \sum_{j=1}^K \mu_j^i n_j^* - \sum_{k=1}^{m_1} \kappa_k^i a_k^* - \Xi_{b_i^*}^2(\mathbf{n}, \mathbf{a}, \mathbf{b}, \mathbf{a}^*, \mathbf{b}^*), \quad i = 1, \dots, m_2$$

# Customer of thermodynamics: Model of BR, algorithm

- Identification of crucial biochemical processes
- Modified LoMA
- Parameter setting
- FEM implementation



# Femur in a healthy individual, simulation



Standard serum levels of considered biochemical factors corresponding to a *healthy state/individual*: estradiol  $50 \frac{\text{pg}}{\text{ml}}$ , PTH  $34 \frac{\text{pg}}{\text{ml}}$ , RANKL  $46.2 \frac{\text{pg}}{\text{ml}}$ , OPG  $36 \frac{\text{pg}}{\text{ml}}$ , and NO levels correspond to intake of  $0.044 \frac{\text{mg}}{\text{kg}}$  of nitroglycerin per day. Number of loading cycles is  $N = 10,000$  also corresponding to healthy mechanical stimulus per day

# Predictions and observations

Comparison of prediction of BMD changes from mechano-chemical (CIT) model to data found in literature.

	hyperPTH	post-menopausal osteoporosis	estradiol 17.5 $\frac{\mu\text{g}}{\text{ml}}$	running 6 mi/day
$BMD_{ind}$	-10.4%	-5.6%	< -1%	+16.2%
literature	-(7 - 15)%	-5.7%	< -1%	+14.1%

# Conclusions

- Can coupling analysis be carried out outside of linear regime (close to equilibrium) when majority of chemical processes are considered to be far from equilibrium? How?
- (partners) Multi-disciplinary approach is needed for many problems - non-equilibrium thermodynamics can be used with success
- (partners&customers) Bridging of this gap with non-equilibrium thermodynamics
- Experimental verification of mechano-chemical coupling

# A nonlinear coupling of chemical kinetics with mechanics

V. Klika<sup>1,2</sup>, M. Grmela<sup>3</sup>

<sup>1</sup>Institute of Thermomechanics of the AS CR, CR  
klika@it.cas.cz

<sup>2</sup>Dept. of Mathematics, FNSPE, Czech Technical University in Prague, CR

<sup>3</sup>Chemical Engineering, Ecole Polytechnique, Montreal, Canada

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