Part II

Continuum limit for 3D mass-spring networks and discrete Korn's inequality.

Joint work with M. Berezhnyy (Ph.D. student) J.Mech. Phys. Solids, v. 54, 2006.

Starting point: a discrete model.

Goal: derive and justify the corresponding continuum model – readily amenable for mathematical analysis (Unlike in part I).

Classical work: M. Born, K. Huang. "Dynamical theory of crystal solids, 1954." A formal derivation of continuum linear elasticity from a periodic mass-spring model with central, pair-wise interaction.

Key ingredient: Cauchy-Born (CB) rule: linear displacement at the boundary of a monoatomic crystal $\Rightarrow$ all atoms follow a linear interpolation of this displacement.

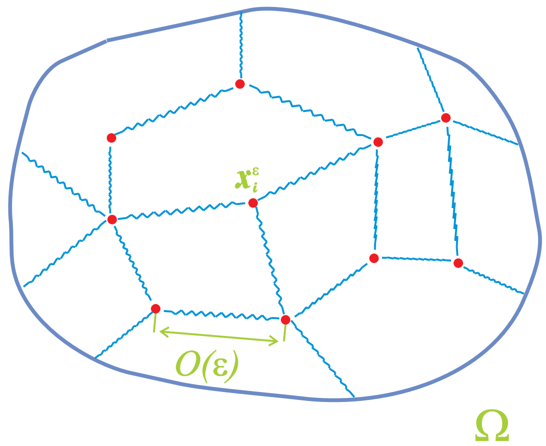
Validity of CB rule under various assumptions: Blanc, Le Bris, Lions, 2002. Hypothesis: **macro**scopic displacement equals **micro**scopic one.

Quasi-Continuum approach (QC), W.E, P. Ming, 2004, ...

Failure of CB rule: Examples of 2D mass-spring lattices, special values of lattice parameters – Le Dret, 1987, Friesecke, Theil, 2002. Mathematical justification of limits of validity of CB is necessary.

Our work: a non-periodic 3D array of point masses connected by linear springs.
– a general geometric condition on a non-periodic array of particles is introduced
– discrete Korn's inequality, which allows to justify the limit, is proved for such arrays. Korn's constant – in terms of lattice parameters – controls instabilities.

The discrete problem

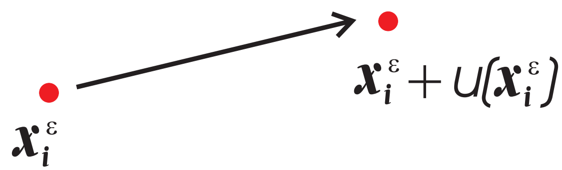


$\Omega \subset \mathbb{R}^3$; N particles with coordinates x_i^ε, $i = 1, \dots, N$ – large.
$\varepsilon = N^{-1/3}$ – small parameter.

Distances between neighboring particles are $O(\varepsilon)$:

$$c_2\varepsilon \leq |x_i^\varepsilon - x_i^\varepsilon| \leq c_1\varepsilon, \qquad c_1, c_2 > 0.$$

Each particle has mass $m_i^\varepsilon = M_i\varepsilon^3$, and less than k neighbors connected by elastic springs. $M_i > 0$ and k do not depend on ε.



u_i^ε – the displacement of i-th particle. The displacements are small in the sense

$$|u_i^\varepsilon - u_j^\varepsilon| \leq c\varepsilon.$$

This is a crucial assumption; its violation may result in instabilities even for quadratic springs analogous to Friesecke, Theil on 2D.

Quadratic springs: elastic energy is

$$\left\langle C_\varepsilon^{i,j}\left(u_i^{(\varepsilon)}-u_j^{(\varepsilon)}\right),\ \left(u_i^{(\varepsilon)}-u_j^{(\varepsilon)}\right)\right\rangle,$$

where $< \cdot, \cdot >$ is a dot product in $\mathbb{R}^3$. Central interaction

$$C_\varepsilon^{i,j}\left(u_i^{(\varepsilon)}-u_j^{(\varepsilon)}\right)=K_\varepsilon^{ij}\left\langle \frac{u_i^{(\varepsilon)}-u_j^{(\varepsilon)}}{x_i^{(\varepsilon)}-x_j^{(\varepsilon)}},\ e_{ij}^\varepsilon\right\rangle,$$

K_ε^{ij} – a (scalar) spring constant.

Intensity of the elastic interaction $K_\varepsilon^{ij}=K^{ij}\varepsilon^2$,
$0<K_1<K^{ij}<K_2$, K_1, K_2 are independent of ε.

Potential energy of the network is

$$H(u_1^\varepsilon,\ldots,u_N^\varepsilon)=H_0+\frac{1}{2}\sum_{i,j}\left\langle C_\varepsilon^{i,j}\left(u_i^{(\varepsilon)}-u_j^{(\varepsilon)}\right),\ \left(u_i^{(\varepsilon)}-u_j^{(\varepsilon)}\right)\right\rangle,$$

H_0 – an arbitrary constant.

Number of terms in the sum

$$H(u_1^\varepsilon, \ldots, u_N^\varepsilon) = H_0 + \frac{1}{2} \sum_{i,j} \left\langle C_\varepsilon^{i,j} \left(u_i^{(\varepsilon)} - u_j^{(\varepsilon)} \right), \ \left(u_i^{(\varepsilon)} - u_j^{(\varepsilon)} \right) \right\rangle ,$$

is $O(\varepsilon^{-3})$, $u_i^\varepsilon \sim \varepsilon$, hence, this scaling implies finite energy.

For the unique equilibria clamp "near boundary particles" in ε–neighborhood of $\partial\Omega$:

$$x_i^{(\varepsilon)}, \quad i = 1, \ldots, M, \quad M = O(\varepsilon^2).$$

Motion of the network is described by the system of $3N$ equations:

$$m_i^{(\varepsilon)} \frac{\partial^2}{\partial t^2} u_i^{(\varepsilon)} = -\nabla u_i^{(\varepsilon)} H(u_1^{(\varepsilon)}, \ldots, u_N^{(\varepsilon)}), \quad i = 1, \ldots, N.$$

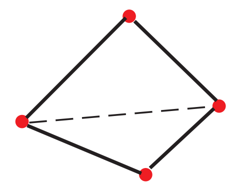
IC: $\quad u_i^{(\varepsilon)}(0) = 0, \ \frac{\partial}{\partial t} u_i^{(\varepsilon)} = a_i^{(\varepsilon)}, \ i = 1, \ldots, N;$

BC: $\quad u_i^{(\varepsilon)}(t) \equiv 0, \ \ t > 0, \ i = 1, \ldots, M.$

Initial velocities $a_i^{(\varepsilon)}$, $i = 1, \ldots, N$ satisfy

$$\sum_i^N m_i^{(\varepsilon)} |a_i^{(\varepsilon)}| \leq C \ \ \text{(Kinetic energy is bounded).}$$

Goal: derive the continuum limit when the network spacing $\varepsilon \to 0$.



a symplex

Def: A network is called a triangulized network if it satisfies the following conditions:

– the points $x_i^{(\varepsilon)}$ partition the domain Ω into simplexes (pyramids) P_ε^α whose edges connect neighboring (interacting) particles and

– angles are uniformly bounded below by $c > 0$ independent of ε (pyramids do not degenerate).

Pyramids are not necessarily identical since the particle array is non-periodic.

In order to study convergence, introduce the linear spline $u_\varepsilon(x)$ corresponding to the discrete vector function $u_i^{(\varepsilon)}$

$$\begin{aligned} u_\varepsilon(x) &= \sum_{i=1}^{N} u_i^{(\varepsilon)} L_\varepsilon^i(x), \\ L_\varepsilon^i(x_k^\varepsilon) &= \delta_{ik}, \quad L_\varepsilon^i \ \text{ is linear.} \end{aligned}$$

Key technical point: discrete Korn's inequality:

$$\text{(K)} \quad \|u_\varepsilon(x)\|^2_{H^1(\Omega)} \leq \bar{C} \sum_{i,j} \left\langle C^{i,j}(u_i^{(\varepsilon)} - u_j^{(\varepsilon)}),\ (u_i^{(\varepsilon)} - u_j^{(\varepsilon)}) \right\rangle,$$

$\bar{C} = \frac{4c_1^3}{3K_1c_2}$; RHS – elastic energy,
$c_1,\ c_2$ – bounds on spacing between neighboring particles,
K_1 – lower bound on spring constant.

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(K) is proved for triangulized networks and it implies convergence of $u_\varepsilon(x)$ to a continuum limit (compactness of $u_\varepsilon(x)$).

If K_1 or c_2 become small, $\bar{C}$ blows up $\Rightarrow$ instabilities a la Friesecke, Theil, no continuum limit.

The continuum limit (linear elasticity), convergence of the splines

$$u^{(\varepsilon)(x,t)} \text{ to } u(x,t).$$

$$\begin{aligned}
&\rho(x)u_{tt} - \frac{\partial}{\partial x_q}\left[a_{npqr}(x)\varepsilon_{np}[u(x,t)]e_r\right] = 0,\ x \in \Omega,\ t > 0,\\
&u(x,t) = 0, \quad x \in \partial\Omega, \quad t \geq 0,\\
&u(x,0) = 0, \quad u_t(x,t) = a(x), \quad x \in \Omega, \quad t = 0.
\end{aligned}$$

$\rho(x)$, $a(x)$ – limiting mass density and initial velocity distribution.
e_r, $r = 1, 2, 3$ – basis in $\mathbb{R}^3$

$a_{npqr}(x)$ are obtained via method of mesocharacteristics from homogenization (L. B., E. Khruslov).

Homogenization techniques (Γ-developments, HMM, mesocharacteristics) are useful in atomic to continuum limits.

Idea of method of Mesocharacteristics:

Mesoscale h: $\varepsilon \ll h \ll \mathrm{diam}(\Omega)$.

K_h^y – a cube centered at $y \in \Omega$, side length h, cover Ω by such cubes.

$E_{K_h^y}$ = (discrete elastic energy + penalty term) – quadratic form for any constant tensor T_{np}

$$E_{K_h^y} = a_{npqr}(y, \varepsilon, h) T_{np} T_{qr}$$

Penalty term forces discrete function $u_i^{(\varepsilon)}$ restricted to K_h^y to be "smooth" (close to a linear one) on scale h – "homogenization" on the mesoscale.

Effective elastic constants at a point $y \in \Omega$ are

$$a_{npqr}(y) = \lim_{h \to 0} \lim_{\varepsilon \to 0} \frac{a_{npqr(y,\varepsilon,h)}}{h^3}.$$

Example: Cubic lattice, connecting springs are:

NN (edges of unit periodicity cell)

NNN(diagonals of the faces of cube)

NNNN (diagonals of the cube).

$$a_{nnnn} = k\left(1 + \sqrt{2} + \frac{4}{9}\sqrt{3}\right),$$

$$a_{nnpp} = a_{npnp} = k\left(\frac{1}{2}\sqrt{2} + \frac{4}{9}\sqrt{3}\right).$$

Coincide with previously known formulas, but now they are justified and limits of validity are attached.

A wide variety of tools is available for linear elasticity PDE.

Current (future work) with L. Truskinovsky (Ecole Polytechnic):

- Establishing the limits of validity of the CB rule for lattices (networks) with geometrical nonlinearities.
- Rigorous mathematical understanding of the continuum and quasi-continuum limit (QC approximation).

QC limit – a continuum model which still contains several atomistic length scales (internal variables, non-local kernels, high derivatives)

e.g. Friesecke, James (2000) – continuum limit for thin films with internal variables.

Conclusions, Part II

- By contrast with part I, continuum (possibly hybrid) models may be advantageous in studies of crystalline solids. Well-developed machinery of PDEs and Calculus of Variations for continuum problems.
- Recent examples of failure of CB rule underline the need for rigorous analysis of the atomistic to continuum limit with emphasis on the limits of validity. In the work L.B., Berezhnoy a classical problem of derivation of continuum elasticity PDEs from a generic 3D array of masses/springs was considered in a rigorous math frameworks of mezocharacteristic approach. Limits of validity are specified.
- The existing math approaches of homogenization theory (mesocharacteristic, Γ-development, HMM) are useful in the derivation of continuum models.