The role of polyconvexity in dynamical problems of thermomechanics

Thanos Tzavaras

Computer, Electrical and Mathematical Science & Engineering

King Abdullah University of Science and Technology KAUST

Cleopatra Christoforou (U. Cyprus)
Myrto Galanopoulou (KAUST)
Sophia Demoulini (Cambridge)
David Stuart (Cambridge)

Outline

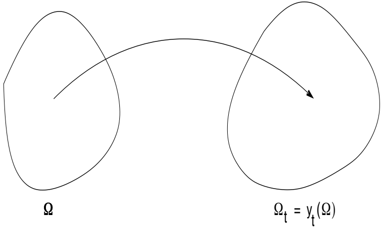
1. the system of polyconvex thermoelasticity
2. Relative entropy and its Applications
3. Variational Approximation
4. lattice models and continuum limits

System of Thermoelasticity

$$
\begin{aligned}
F_t &= \nabla v \\
v_t &= \operatorname{div} S \\
\partial_t(\tfrac{1}{2}|v|^2 + e) &= \operatorname{div}(v \cdot S) + \operatorname{div} Q + r
\end{aligned}
$$

$$
\partial_t \eta - \operatorname{div} \frac{Q}{\theta} \geq \frac{r}{\theta}
$$

motion	$y(t,x)$
velocity	$v = \dfrac{\partial y}{\partial t}$
deformation gradient	$F = \nabla y$
involutive constraint	$\operatorname{curl} F = 0$



theory of thermoviscoelasticity : free energy $\psi = \psi(F, \theta)$

$$
\begin{aligned}
S &= \frac{\partial \psi}{\partial F}(F, \theta)\,, \\
\eta &= -\frac{\partial \psi}{\partial \theta}(F, \theta)\,, \\
e &= \psi + \theta \eta\,.
\end{aligned}
$$

total stress $S_{tot} = S + \mu \nabla v$ heat flux $Q = \kappa \nabla \theta$

$\mu = \mu(F, \theta) \geq 0$ $\kappa = \kappa(F, \theta) \geq 0$

Coleman - Noll '63, Coleman - Mizel '64

system of thermoviscoelasticity in Lagrangean coordinates

$$
\begin{aligned}
F_t &= \nabla v \\
v_t &= \operatorname{div}(S + \mu \nabla v) \\
\partial_t\left(\tfrac{1}{2}|v|^2 + e\right) &= \operatorname{div}(v \cdot S + v \cdot \mu \nabla v) + \operatorname{div}(\kappa \nabla \theta) + r
\end{aligned}
$$

$$
\partial_t \eta - \operatorname{div} \frac{\kappa \nabla \theta}{\theta} = \frac{1}{\theta^2}\kappa |\nabla \theta|^2 + \frac{1}{\theta}\mu |\nabla v|^2 + \frac{r}{\theta} \quad \geq \quad \frac{r}{\theta}
$$

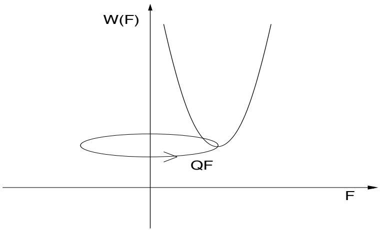
- **Material frame indifference**

$$\psi(QF, \theta) = \psi(F, \theta) \quad \forall\ Q \in \mathcal{O}^3$$

- **Realizibility of mechanical motions**

to avoid interpenetration of matter impose (at least) positivity of the Jacobian

$$\det F > 0$$



$$W(F) \to \infty \quad \text{as} \quad \det F \to 0$$

It is too restrictive to take $W(F)$ convex

The problem of stabilization

The local state (F, η) is a state of thermal equilibrium under a given force-temperature pair (S, θ) if

- the Cauchy stress $T = \frac{1}{\det F} F S^T$ is symmetric
- the inequality holds

$$\lambda(F^*, \eta^*) > \lambda(F, \eta) \qquad \forall \ (F^*, \eta^*) \neq (F, \eta) \text{ with } F^\star = GF$$

  with G symmetric positive definite

where

$$\lambda(F, \eta) = e(F, \eta) - S \cdot F - \eta\theta$$

$\lambda =$ internal energy - potential energy of contact forces - thermal potential energy.

Recall polar decomposition: if $detF \neq 0$ then $F = QU$, Q rotation, $U > 0$ symmetric

Coleman-Noll '59 - following Gibbs 1875

Coleman-Noll '59 show that the free energy $\psi = e - \theta\eta$ for a thermoelastic theory determined by

$$\psi = \psi(F, \theta)$$

when (F, θ) is a state of thermal equilibrium has to satisfy

$$\psi(F^*, \theta^*) - \psi(F, \theta) - \frac{\partial \psi}{\partial F}(F, \theta) \cdot (F^* - F) - \frac{\partial \psi}{\partial \theta}(F^*, \theta^*)(\theta^* - \theta) > 0$$

$\forall \ (F^*, \theta^*) \neq (F, \theta)$ with $F^\star = GF$, with $G > 0$ symmetric

This implies

$$\psi_{\theta\theta} < 0$$

but does not imply

$$\psi_{FF} > 0$$

Notions from Elastostatics

$$\min_{y \in W^{1,\infty}} I[y] = \int_\Omega W(\nabla y)\, dx$$

$\Phi(F)$ is a null-Lagrangean iff

$$\begin{aligned} \int_\Omega \Phi(\nabla y + \nabla \phi)\, dx = \int_\Omega \Phi(\nabla y) dx \quad \forall\ y \in W^{1,p}\,,\ \phi \in C_c^\infty \\ \iff \quad \partial_\alpha \left(\frac{\partial \Phi}{\partial F_{i\alpha}}(\nabla y) \right) = 0 \quad \text{in } \mathcal{D}' \\ \iff \quad \Phi(F) = A : F + B : \operatorname{cof} F + c \det F \end{aligned}$$

If $\Phi(\nabla y)$ is null-Lagrangean then it is weakly continuous in $W^{1,p}$.

J. Ball 77, J. Ericksen 62

$W(F)$ is polyconvex

$$W(F) = g(F, \operatorname{cof} F, \det F) = g \circ \Phi(F) \qquad \text{with } g(\Xi) \text{ convex}$$

Transport Identities

$$\frac{\partial}{\partial t}\det F = \frac{\partial}{\partial x^\alpha}\big((\operatorname{cof} F)_{i\alpha} v_i\big)$$
$$\frac{\partial}{\partial t}(\operatorname{cof} F)_{k\gamma} = \frac{\partial}{\partial x^\alpha}\big(\epsilon_{ijk}\epsilon_{\alpha\beta\gamma}F_{j\beta}v_i\big)$$

connected to null-Lagrangians $\Phi(F) = (F, \operatorname{cof} F, \det F)$

$$\partial_\alpha\left(\frac{\partial\Phi}{\partial F_{i\alpha}}(\nabla y)\right) = 0 \quad \text{in } \mathcal{D}'$$

Transport identities

$$\partial_t F_{i\alpha} = \partial_\alpha v_i$$
$$\partial_t \Phi^A(F) = \partial_\alpha\left(\frac{\partial\Phi^A}{\partial F_{i\alpha}}\, v_i\right) \quad A = 1, ..., 19$$

These identities describe the transport and stretching of the elementary volume and areas and have offered a lot of understanding in the dynamics of isothermal elasticity

T. Qin 98, Demoulini-Stuart-T '01, '12, Dafermos '06, Lattanzio-T. '06

The Polyconvex Thermoelasticity System

$$\psi(F,\theta) = g(\Phi(F),\theta) \qquad \text{polyconvexity hypothesis}$$

$$\begin{aligned}
\partial_t \Phi(F)^A &= \partial_\alpha \left(\frac{\partial \Phi^A}{\partial F_{i\alpha}}(F)\, v_i \right) \\
\partial_t v &= \partial_\alpha \Big(S^A(\Phi(F),\theta)\, \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \Big) \\
\partial_t \left(\tfrac{1}{2}|v|^2 + \bar{e}(\Phi(F),\theta) \right) &= \partial_\alpha \Big(v_i\, S^A(\Phi(F),\theta)\, \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \Big) + r \\
\mathrm{curl} F &= 0
\end{aligned}$$

where $S^A = \frac{\partial g}{\partial \xi^A}(\xi,\theta)$

augmented system

$$\partial_t \xi^A = \partial_\alpha \left(\frac{\partial \Phi^A}{\partial F_{i\alpha}}(F)\, v_i \right)$$

$$\partial_t v = \partial_\alpha \Big(S^A(\xi,\theta)\, \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \Big)$$

$$\partial_t \left(\tfrac{1}{2}|v|^2 + \bar{e}(\xi,\theta) \right) = \partial_\alpha \Big(v_i\, S^A(\xi,\theta)\, \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \Big) + r$$

system in $\Big(v, \underbrace{(F, Z, w)}_{\xi}, \theta \Big)^T$ variables.

Using the null-Lagrangian property $\partial_\alpha \left(\frac{\partial \Phi}{\partial F_{i\alpha}}(\nabla y) \right) = 0$ one can derive the entropy production identity for smooth solutions of the augmented system

$$\partial_t \bar{\eta}(\xi,\theta) = \frac{r}{\theta}$$

Properties of the extension

(a) The augmented system is symmetrizable under the hypothesis

$$g_{\xi\xi}(\xi,\theta) > 0\,, \quad g_{\theta\theta}(\xi,\theta) < 0$$

(b) The adiabatic, polyconvex, thermoelastsicity (APT) system may be viewed as a constrained evolution:

$$\xi(\cdot,0) = \Phi(F(\cdot,0)) \quad \Longrightarrow \quad \xi(\cdot,t) = \Phi(F(\cdot,t)) \;\; \forall t$$

(c) Recall and compare to the property

$$F(\cdot,0) = \nabla y(\cdot,0) \quad \Longrightarrow \quad F(\cdot,t) = \nabla y(\cdot,t) \;\; \forall t$$

Symmetrization of Hyperbolic Systems

$$\begin{cases} \partial_t A(u) + \partial_\alpha F_\alpha(u) = 0 & (\star) \\ \\ \partial_t \eta(u) + \partial_\alpha q_\alpha(u) = 0 \end{cases}$$

multiplier $G(u)^T$

$$G \cdot \nabla A = \nabla \eta \quad \iff \quad \nabla G^T \nabla A = \nabla A^T \nabla G$$

$$G \cdot \nabla F_\alpha = \nabla q_\alpha \quad \iff \quad \nabla G^T \nabla F_\alpha = \nabla F_\alpha^T \nabla G$$

$$\underbrace{\nabla G^T \nabla A}_{symmetric} \, \partial_t u + \nabla G^T \nabla F_\alpha \, \partial_\alpha u = 0$$

System $(\star)$ is symmetrizable if

$$\nabla G^T \nabla A = \nabla^2 \eta - G \cdot \nabla^2 A > 0$$

equivalently, if we express

$$H \circ A(u) = \eta(u) \qquad H(v) \text{ is convex}$$

$$\partial_t A(u) + \partial_\alpha F_\alpha(u) = \varepsilon \partial_\alpha \big(B(u) \partial_\alpha u \big)$$

$$\partial_t \eta(u) + \partial_\alpha q(u) = \varepsilon \partial_\alpha \big(G(u) \cdot B(u) \partial_x u \big) - \varepsilon \nabla G(u) \partial_\alpha u \cdot B(u) \partial_\alpha u$$

Main Assumption

$$\nabla G^T \nabla A = \nabla^2 \eta - G \cdot \nabla^2 A > 0$$

Relative entropy

$$\eta(u) - \eta(\bar{u}) - G(\bar{u}) \cdot (A(u) - A(\bar{u})) = H\big(A(u) | A(\bar{u})\big)$$

Compare two solutions u and $\bar{u}$ of the hyperbolic-parabolic system

$$
\begin{aligned}
\partial_t \Big[H\big(A(u) | A(\bar{u})\big) \Big] &+ \partial_\alpha \Big(q_\alpha(u|\bar{u}) + \varepsilon J_\alpha \Big) \\
&\qquad + \varepsilon \sum_\alpha \partial_\alpha (u - \bar{u}) \cdot \nabla G(u)^T B(u) \partial_\alpha (u - \bar{u}) \\
= -\Big(\partial_\alpha G(\bar{u}) \Big) &\cdot \Big[F_\alpha(u) - F_\alpha(\bar{u}) - \nabla F_\alpha(\bar{u}) \big(\nabla A(\bar{u}) \big)^{-1} (A(u) - A(\bar{u})) \Big] \\
+ \varepsilon \sum_i Q_i &
\end{aligned}
$$

where

$$
\begin{aligned}
Q_i &\sim (\partial_\alpha u - \partial_\alpha \bar{u}) \cdot (u - \bar{u}) \\
Q_j &\sim |u - \bar{u}|^2
\end{aligned}
$$

Convergence of zero-viscosity limit when $\bar{u}$ is smooth.

Application: From thermoviscoelasticity to adiabatic thermoelasticity

Thm Under Hypotheses of Gibbs thermodynamic stability, L^p growth for $e(F,\theta)$, if $\bar{U}$ is a smooth solution of adiabatic thermoelasticity, and

$$0 < \mu = \mu(F,\theta) \le \mu_0 \,, \quad 0 < \kappa = \kappa(F,\theta) \le k_0 \theta$$

then

$$\sup_{t \in (0,T)} \int I(U^{\mu,k}(t) | \bar{U}(t)) dx \to 0 \qquad \text{as } \mu_0, k_0 \to 0+ \ .$$

Christoforou, T. 2016

entropy and relative entropy

$$H(U) = -\eta(F,\theta)$$

$$
\begin{aligned}
H(U) - H(\bar U) - G(\bar U)\cdot(A(U) - A(\bar U)) \\
&= (-\eta) - (-\bar\eta) - \left(\frac{\bar\Sigma}{\bar\theta}, \frac{\bar v}{\bar\theta}, -\frac{1}{\bar\theta}\right)\cdot\left(F - \bar F, v - \bar v, e + \tfrac12 v^2 - \bar e - \tfrac12 v^2\right) \\
&= \tfrac{1}{\bar\theta}\left(\delta e - \bar\theta\delta\eta - \bar\Sigma : \delta F - \bar v \delta v\right) \\
&= \frac{1}{\bar\theta}\Big(\underbrace{\psi(F,\theta|\bar F,\bar\theta) + (\eta - \bar\eta)(\theta - \bar\theta)}_{\lambda(F,\theta|\bar F,\bar\theta)}\Big) + \tfrac12 (v - \bar v)^2
\end{aligned}
$$

Remarks

$\lambda(F,\theta|\bar F,\bar\theta) > 0$ is thermal stability condition proposed by Coleman-Noll '59

$$\nabla^2 H(U) - G(U)\cdot\nabla^2 A(U) > 0 \quad \Leftrightarrow \quad \psi_{FF} > 0, \quad \eta_\theta > 0$$

The system of polyconvex thermoelasticity

Polyconvex Thermoelasticity $\psi(F,\theta) = \hat{\psi}(F, \operatorname{cof} F, \det F, \theta)$

Thm Under Hypotheses

$$\hat{\psi}_{\xi\xi}(\xi,\theta) > 0 \qquad \hat{\psi}_{\theta\theta}(\xi,\theta) < 0$$

L^p growth for $\hat{e}(\xi,\theta)$, if $\bar{U}$ is a smooth solution of adiabatic polyconvex thermoelasticity, and

$$0 < \mu = \mu(F,\theta) \le \mu_0\,, \quad 0 < \kappa = \kappa(F,\theta) \le k_0\theta$$

then

- convergence from thermoviscolasticity to adiabatic thermoelasticity as $\mu_0, k_0 \to 0$
- or from thermoviscoelasticity to thermoelasticity as $\mu_0 \to 0$, k_0 constant.
- weak-strong uniqueness for measure-valued solutions

Galanopoulou - Christoforou - T. 2018 , Koumatos-Spirito 2019 isothermal quasiconvex

Variational Approximation

Isothermal dynamic elasticity has the following properties:

- Variational approximation connected to viewing the problem

$$\partial_{tt} y = -\frac{\delta}{\delta y}\Big(\int W(\nabla y) dx \Big)$$

discretize the evolution in time.

- In 1-d this approximation yields entropic weak solutions that satisfy the entropy inequality for any convex entropy

Motivation Demoulini-Stuart- T. '99, '01, Cavalletti-Sedjro-Westdickenberg '15

Question What is the analog for the non-isothermal case ?

Given a free energy function $\psi = \psi(F, \theta)$ define the Legendre transform

$$e(F, \eta) = \sup_{\theta} \Big(\theta \eta + \psi(F, \theta) \Big)$$

$e(F, \eta)$ is computed by

$$e(F, \eta) = \psi(F, \theta^*) + \theta^* \eta \quad \text{where } \theta^*(\eta) \text{ is such that } \eta = -\tfrac{\partial \psi}{\partial \theta}(F, \theta^*)$$

If $\psi_{\theta\theta} < 0$ then $e_{\eta\eta} > 0$. No convexity is assumed in F.

- The thermodynamic potential $e(F, \eta)$ - internal energy - is the Legendre dual of $-\psi(F, \theta)$ - Helmholtz free energy

Consider the augmented system expressed in the (v, ξ, η) variables

$$\partial_t \xi^A = \partial_\alpha \left(\frac{\partial \Phi^A}{\partial F_{i\alpha}}(F)\, v_i \right)$$

$$\partial_t v = \partial_\alpha \Big(\frac{\partial \bar{e}}{\partial \xi^A}(\xi, \eta)\, \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \Big)$$

$$\partial_t \left(\tfrac{1}{2}|v|^2 + \bar{e}(\xi, \eta) \right) = \partial_\alpha \Big(v_i\, \frac{\partial \bar{e}}{\partial \xi^A}(\xi, \eta)\, \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \Big) + r$$

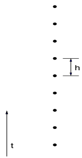
Entropy identity

$$\partial_t \bar{\eta} = \frac{r}{\frac{\partial \bar{e}}{\partial \eta}(\xi, \eta)}$$

under the hypothesis $\bar{e}(\xi, \eta)$ convex in ξ and in η which renders the system symmetrizable.

Consider the minimization problem: Given (v^0, ξ^0, η^0)

$$\min \int_{\mathbb{T}^3} \left(\frac{1}{2} |v - v^0|^2 + \bar{e}(\xi, \eta) \right) \, dx$$



over the affine subspace

$$\mathcal{C} := \Big\{ (v, \underbrace{F, Z, w}_{\xi}) : \mathbb{T}^3 \to \mathbb{R}^{22} \ \text{ subject to the constraints}$$

$$\left. \begin{aligned} \frac{\xi - \xi^0}{h} &= \partial_\alpha \Big(\frac{\partial \Phi^A}{\partial F_{i\alpha}}(F^0) \, v_i \Big) \\ \frac{\eta - \eta^0}{h} &= \frac{r}{\bar{\theta}(\Phi(F^0), \eta^0)} \end{aligned} \qquad \right\}.$$

Under convexity of $\bar{e}(\xi, \eta)$ this problem is solvable and sets-up an iteration scheme with a variational framework in the background.

Euler-Lagrange equations

Computing the variation of the functional, the iterates satisfy

$$\begin{aligned}
\frac{v - v^0}{h} &= \partial_\alpha \Big(\frac{\partial \bar{e}}{\partial \xi^A}(\xi,\eta) \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F^0) \Big) \\
\frac{\xi^A - \xi^{0,A}}{h} &= \partial_\alpha \Big(\frac{\partial \Phi^A}{\partial F_{i\alpha}}(F^0)\, v_i \Big) \\
\frac{\eta - \eta^0}{h} &= \frac{r}{\bar{\theta}(\Phi(F^0), \eta^0)}
\end{aligned}$$

Using convexity of $\bar{e}(\xi,\eta)$

$$\begin{aligned}
&\frac{\left(\frac{1}{2}|v|^2 + \bar{e}(\xi,\eta)\right) - \left(\frac{1}{2}|v^0|^2 + \bar{e}(\xi^0,\eta^0)\right)}{h} + \underbrace{J(v^0, \Phi(F^0), \eta^0 | v, \xi, \eta)}_{\geq 0} \\
&\qquad = \partial_\alpha \Big(v_i \frac{\partial \bar{e}}{\partial \xi^A}(\xi,\eta) \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F^0) \Big) + \frac{\bar{\theta}(\xi,\eta)}{\bar{\theta}(\Phi(F^0), \eta^0)} r
\end{aligned}$$

Under convexity $\bar{e}(\xi, \eta)$ and bounds on $\bar{e}$ and $\frac{\partial \bar{e}}{\partial \Xi}$, $\frac{\partial \bar{e}}{\partial \eta}$ we obtain a Young measure ν and a nonnegative concentration measure $\gamma(dxdt)$ s.t.

$$v^h \rightharpoonup v \quad \text{wk in } L^2, \quad \eta^h \rightharpoonup \eta \quad \text{wk in } L^r$$
$$(F^h, Z^h, w^h) \rightharpoonup (F, \operatorname{cof} F, \det F) \quad \text{wk in } L^p \times L^q \times L^r$$

where $F = \langle \nu, \lambda_F \rangle$, $v = \langle \nu, \lambda_v \rangle$, $\eta = \langle \nu, \lambda_\eta \rangle$ satisfy

Dissipative measure-valued solution

$$\partial_t \Phi^A(F) = \partial_\alpha \left(\frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) v_i \right)$$

$$\partial_t v_i = \partial_\alpha \langle \nu, S_{i\alpha}(\lambda_F, \lambda_\theta) \rangle$$

$$\partial_t \Big\langle \nu, \bar{\eta}(\Phi(\lambda_F), \lambda_\theta) \Big\rangle \geq \Big\langle \nu, \frac{r}{\lambda_\theta} \Big\rangle$$

Integrated Energy inequality

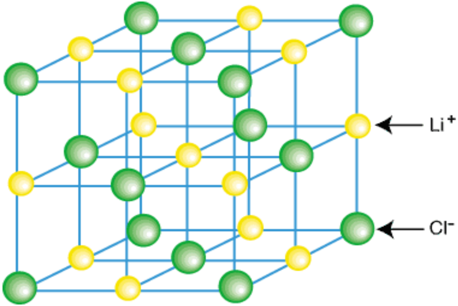
$$\partial_t \int \left\langle \nu, \tfrac{1}{2} |\lambda_v|^2 + \bar{e}(\Phi(\lambda_F), \lambda_\theta) \right\rangle dx + d\gamma(x,t) \leq 0$$

Geometric transport identities and null-Lagrangeans are weakly stable.

- Thm. measure-valued weak versus strong uniqueness theorem
- Corollary Convergence of the variational scheme to smooth solutions of adiabatic thermoelasticity.

Galanopoulou - Christoforou - T. 2018

Lattice models and their continuum limits



WORK IN PROGRESS WITH S. DEMOULINI - D. STUART

Ionic lattices and deformation energy

Charges $\{q_n\}_{n\in\Lambda}$ located in equilibrium $\{\mathbf{X}(n) = \epsilon n\}_{n\in\Lambda}$

$$\Lambda = \mathbb{Z}^d \quad \text{or} \quad \Lambda = \Lambda_N = \{0, \dots (N-1)\}^d$$

Assume charges all $+q$ or $-q$ on lattice.
Displaced to locations $\{\mathbf{x}(n) \in \mathbb{R}^d\}_{n\in\Lambda}$.

- Short range (nearest neighbour) interactions

$$V_s = \sum_{n\in\Lambda} \epsilon^d W(\partial^\epsilon \mathbf{x}(n))$$

- Long range interactions from electrostatic forces

$$V_{el} = q^2 \Big[\sum_{pos-pos} K(\mathbf{x}(n), \mathbf{x}(n')) + \sum_{neg-neg} K(\mathbf{x}(n), \mathbf{x}(n')) - 2 \sum_{pos-neg} K(\mathbf{x}(n), \mathbf{x}(n')) \Big]$$

As a model problem consider a fixed background positive charge distribution

$$V_{el} = \frac{1}{2} \iint \Big(\rho_B(\mathbf{x}) - q \sum \delta(\mathbf{x} - \mathbf{x}(n))\Big) K(\mathbf{x}, \mathbf{x}') \\ \Big(\rho_B(\mathbf{x}') - q \sum \delta(\mathbf{x}' - \mathbf{x}(n))\Big) d\mathbf{x} d\mathbf{x}'$$

- This could arise if positive ions are very heavy so dynamically frozen
- Assume $K \in C^2$, but keep Coulomb in mind:

$$K(\mathbf{x}(n), \mathbf{x}(n')) = C|\mathbf{x}(n) - \mathbf{x}(n')|^{-1}$$

Euler-Lagrange equations of motion from Lagrangian

$$\mathcal{L}(\mathbf{x}, \dot{\mathbf{x}}) = \sum_n \frac{1}{2} m_n |\dot{\mathbf{x}}(n)|^2 - V_s - V_{el}$$

$$\begin{aligned} m_n \ddot{\mathbf{x}}_a(n) &= \epsilon^{d-1} \sum_{j=1}^{d} \Big(\sigma_{aj}(\partial_j^\epsilon \mathbf{x}(n)) - \sigma_{aj}(\partial_j^\epsilon \mathbf{x}(n - \iota_j)) \Big) \\ &\quad - q \int \partial_{x_a} K(\mathbf{x}(n), \mathbf{x}') \Big(\rho_B(\mathbf{x}') - q \sum \delta_{\mathbf{x}(n)}(\mathbf{x}') \Big) d\mathbf{x}' \end{aligned}$$

$$|\Lambda_N| = N^d \qquad \text{(Number of lattice sites/particles)}$$

$$\epsilon = \frac{2\pi}{N} \qquad m_n = \epsilon^d \rho_0 \qquad q = \epsilon^d \rho_{el}$$

Blanc-LeBris-Lions formalism gives expected continuum deformation energies in terms of assumed continuum deformation $\{X \to y(X)\}_{X \in [0,2\pi]^d}$

$$V_s \rightsquigarrow \int W(\frac{\partial y}{\partial X}) dX$$

$$V_{el} \rightsquigarrow \frac{1}{2} \iint \left(\rho_B \det \frac{\partial y}{\partial X} - \rho_{el}\right) K(y(X), y(X')) \times \left(\rho_B \det \frac{\partial y}{\partial X'} - \rho_{el}\right) dX dX'$$

This leads to the evolution equation

$$\rho_0 \frac{\partial^2 y_i}{\partial T^2} = \frac{\partial}{\partial X_\alpha}\Big(\sigma_{i\alpha}(\frac{\partial y}{\partial X})\Big) - \rho_{el}\int \partial_{1a} K(y(X), y(X'))\big(\rho_B \det \frac{\partial y}{\partial X'} - \rho_{el}\big) dX'$$

$$\sigma_{i\alpha}(F) = \frac{\partial W}{\partial F_{i\alpha}} \qquad F_{i\alpha} = \frac{\partial y_i}{\partial X_\alpha}$$

$$\partial_{1a} K(y,z) = \frac{\partial}{\partial y_a} K(y,z)$$

- The additional term is of form expected from Coulomb force law, and arises after some cancellations in deriving the Euler-Lagrange equations
- The additional term in the equation of motion is lower order so existence of local classical solutions not expected to be an issue.

These isothermal models are equipped with relative energy identity

- one proves a measure-valued weak versus strong uniqueness theorem for the anticipated limit model
- In second step one shows that the discrete lattice model has uniform bounds in energy norm
- A soft analysis indicates that the lattice model converges to a dissipative mv solution as lattice size tends to zero.
- The mv-weak vs strong uniqueness then guarantees that so long as the limit has a smooth solution the approximate solution converges to the smooth solution.