CIMPA Research School : Data Science for Engineering and Technology
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Bregman divergences
a basic tool for pseudo-metrics building for data structured by physics

6a- Bregman divergences from potentials

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Building generating functions for BD applied to physical data

The goals

- Exploit the a priori information gained by the knowledge about the physics
- Take into account physical constraints
- Non-blind processing of heterogeneous data (multiphysics)
- Build appropriate features characterizing physical data fields

The means

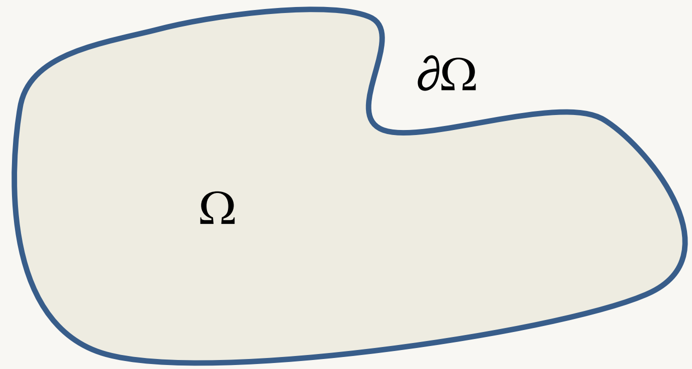
- Take advantage of potentials, energies or dissipations arising from the equations fulfilled by the data
- Enrich the data with (physically) dual variables
- Use the additivity property of the various Bregman divergence notions

Potentials for physical fields data

Data governed by a linear symmetric PDE

$$u \in V,\ \ a(u,v) = l(v) \quad \forall v \in V_0$$

$$a(u,v) = \int_\Omega A(u(x),v(x))dx$$



a symmetric bilinear form on $U(\Omega)$x$U(\Omega)$,
l linear form on U
$V \subset U$ space of admissible fields (Dirichlet boundary conditions on parts of $\partial\Omega$)
V_0 its tangent space

a continuous and coercive
l continuous

$\longrightarrow$

$$u = \underset{V}{\arg\min}\ P(v) = \frac{1}{2}a(v,v) - l(v)$$

$D_A(u(x),v(x)) \geq 0$ $\quad$ 0 only if $u(x) = v(x)$
$D_a(u,v) \geq 0$ $\quad$ 0 only if $u = v$

$$D_A(u(x),v(x)) = A\big(u(x)-v(x),u(x)-v(x)\big)$$
$$D_a(u,v) = a(u-v,u-v)$$

Potentials for physical fields data

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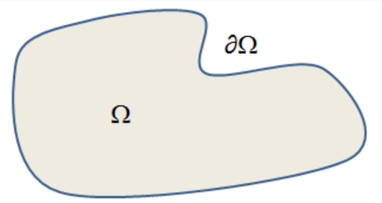

Physics	U space	Energy or dissipation density A
Scalar conduction or diffusion (thermal, electrical, Darcean flow, incompressible Stokes flow)	$H^d(\Omega)$	$\underline{\underline{k}}.\nabla u.\nabla u$
Helmholtz Equation	$H^1(\Omega)$	$\nabla u.\nabla u - k^2 u^2$
Elasticity	$H^1(\Omega)^3$	$\underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\varepsilon}}(u) : \underline{\underline{\varepsilon}}(u)$

Non linear Fluid Dynamics

For Navier-Stokes equation

The kinetic energy $J\left(\mathbf{v}(x)\right) = \rho \left\| \mathbf{v} \right\|^2$

The enstrophy $J\left(\mathbf{v}(x)\right) = \rho \left\| rot\ \mathbf{v} \right\|^2$

Generating functions in thermomechanics for standard generalized materials (I)

Description of the local thermodynamic state

Local thermodynamic state variables (ε, T, α)

ε Deformation or strain
T temperature
α (hidden) internal variables

$$P = \sigma : \dot{\varepsilon} + S\dot{T} + A.\dot{\alpha}$$

Dual variables defined through the power production density (σ, S, A)

σ stress
S Entropy
A Thermodynamic force

Generalized Standard Materials

Formulation of the constitutive equation via <u>two</u> convex potentials

Free or Gibbs energy $\varphi(\varepsilon, \alpha, T)$ ⟶ State laws $\sigma = \frac{\partial \varphi}{\partial \varepsilon}, S = -\frac{\partial \varphi}{\partial T}, A = -\frac{\partial \varphi}{\partial \alpha}$

Pseudo-potential of dissipation $\mathcal{D}(\dot{\alpha})$ ⟶ Evolution law $A \in \partial \mathcal{D}(\dot{\alpha})$ or $\dot{\alpha} \in \partial \mathcal{D}^*(A)$

Generating functions in thermomechanics for standard generalized materials (II)

Incremental Euler implicit constitutive equations

$$\sigma+\Delta\sigma=\frac{\partial\varphi}{\partial\varepsilon}[\varepsilon+\Delta\varepsilon,\alpha+\Delta\alpha],A+\Delta A=-\frac{\partial\varphi}{\partial\alpha}[\varepsilon+\Delta\varepsilon,\alpha+\Delta\alpha],A+\Delta A=\frac{\partial\mathcal{D}}{\partial\dot{\alpha}}\left(\frac{\Delta\alpha}{\Delta t}\right)$$

↓

Pair of conjugate variables
(primal,dual)

$$(\sigma+\Delta\sigma,\varepsilon+\Delta\varepsilon),(A+\Delta A,\alpha+\Delta\alpha)$$

We can the use as the generating function any combination $\varphi+\chi\mathcal{D}\quad\chi\geq 0$

$$D_{\varphi+\chi\mathcal{D}}(\Delta e_1,\Delta e_2)=\varphi(\varepsilon+\Delta\varepsilon_1,A+\Delta A_1)-\varphi(\varepsilon+\Delta\varepsilon_2,A+\Delta A_2)+\chi\mathcal{D}\left(\frac{\Delta\alpha_1}{\Delta t}\right)-\chi\mathcal{D}\left(\frac{\Delta\alpha_1}{\Delta t}\right)$$
$$-(\sigma+\Delta\sigma_2):(\Delta\varepsilon_1-\Delta\varepsilon_2)+\frac{\chi+\Delta t}{\Delta t}(A_2+\Delta A_2)(\Delta\alpha_1-\Delta\alpha_2)$$

$$BG^s_{\varphi+\chi\mathcal{D}}([\Delta e_1,\Delta p_1],[\Delta e_2,\Delta p_2])=(\Delta\sigma_1-\Delta\sigma_2):(\Delta\varepsilon_1-\Delta\varepsilon_1)+\frac{\chi+\Delta t}{\Delta t}\langle\Delta A_1-\Delta A_2,\Delta\alpha_1-\Delta\alpha_2\rangle$$

Generating functions in thermomechanics for standard generalized materials (III)

Phenomenon	Generating function	Symmetrized Bregman gap
Scalar conduction or diffusion	Dissipation function	$\frac{1}{2}\int_\Omega K\nabla(u_1-u_2).\nabla(u_1-u_2)$
Linear elasticity	Elastic energy	$\frac{1}{2}\int_\Omega C:\varepsilon(u_1-u_2):\varepsilon(u_1-u_2)$
Non-linear elasticity	Elastic energy (if convex)	$\int_\Omega(\Delta\sigma_1-\Delta\sigma_2):(\Delta\varepsilon(u_1)-\Delta\varepsilon(u_2))$
Hyper-elasticity	Polyconvex elastic energy (variables : cofactors of *F*)	$\int_\Omega(T_1-T_2):(M_1-M_2)+(cT_1-cT_2):(N_1-N_2)$ $+\int_\Omega(p_1-p_2)(d_1-d_2)$
Standard Elastoplasticity	Free energy Dissipation Pseudo-potential	$\int_\Omega(1-\chi)(\Delta\sigma_1-\Delta\sigma_2):(\Delta\varepsilon(u_1)-\Delta\varepsilon(u_2))+\chi(\Delta A_1-\Delta A_2):(\Delta\alpha_1-\Delta\alpha_2)$
Contact Friction	Elastic energy Dissipation bi-potential	$\int_\Omega(\Delta\sigma_1-\Delta\sigma_2):(\Delta\varepsilon(u_1)-\Delta\varepsilon(u_2))$ $+\int_{\Gamma_c}-(\rho\sigma_{nn}^1-\rho\sigma_{nn}^2)(\lvert u_t^1\rvert-\lvert u_t^2\rvert)+(\sigma_{nt}^1-\sigma_{nt}^2)(u_t^1-u_t^2)$
Non-standard elastoplasticity	Elastic energy Dissipation bi-potential	$\int_\Omega(1-\chi)(\Delta\sigma_1-\Delta\sigma_2):(\Delta\varepsilon(u_1)-\Delta\varepsilon(u_2))$ $+\chi(\Delta A_1-\Delta A_2):(\Delta\alpha_1-\Delta\alpha_2)$
Thermo-elasticity	Elastic energy Thermal Dissipation	$\frac{1}{2}\int_\Omega C:[\varepsilon(u_1-u_2)-\alpha(T_1-T_2)Id]:[\varepsilon(u_1-u_2)-\alpha(T_1-T_2)Id]$ $\frac{1}{2}\int_\Omega K\nabla(u_1-u_2).\nabla(u_1-u_2)$