Error in constitutive relation for material identification

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Identification of material constitutive properties

Generic problem: Identify (possibly heterogeneous) material parameters from overdetermined data, e.g.:

- kinematic data on the boundary:
- vibrational data (eigenfrequencies, eigenmodes at sensors);
- full-field kinematic response of solid under dynamical excitation...

Identification often based on minimizing a data misfit functional

- (weighted) least squares...;
- Reciprocity residuals (reciprocity gap method, virtual fields method);
- Bayesian approaches;
- Error in constitutive equation (ECR)

Concept of error in constitutive equation (ECR)

• Simplest version of ECR (small-strain linear elasticity):

$$
\mathcal{E}(\boldsymbol{u}, \boldsymbol{\sigma}, \boldsymbol{C}) := \frac{1}{2} \int_{\Omega} (\boldsymbol{\sigma} - \boldsymbol{C} : \boldsymbol{\varepsilon}[\boldsymbol{u}]) : \boldsymbol{C}^{-1} : (\boldsymbol{\sigma} - \boldsymbol{C} : \boldsymbol{\varepsilon}[\boldsymbol{u}]) \, dV
$$

$$
\widetilde{\mathcal{E}}(\boldsymbol{C}) := \min_{\boldsymbol{u} \in \mathsf{KA}, \boldsymbol{\sigma} \in \mathsf{SA}} \mathcal{E}(\boldsymbol{u}, \boldsymbol{\sigma}, \boldsymbol{C})
$$

- $\widetilde{\mathcal{E}}(\mathcal{C})$: Energy-based measure of mismatch between KA and SA spaces for given domain, material and loading \implies mechanically meaningful cost functional.
	- ▷ First introduced for error estimation in FEM [Ladevèze, Leguillon 1983];
	- ▷ Soon also proved useful for identification problems [e.g. Reynier 1990]
	- ▷ Similar ideas independently in EIT [Kohn, Vogelius, McKenney, c. 1990]
	- ▷ Also useful for Cauchy / data completion problems [Andrieux, Ben Abda 2006]
	- ▷ Plasticity, damage... [e.g. Latourte et al. 2007, Marchand et al. 2018]
	- \triangleright Special case of Fenchel error \implies ECR for generalized standard materials
- Time-harmonic formulation for e.g. FE model updating [e.g. Reynier 90; Moine 97; Deraemaeker 01; Banerjee et al. 13; Aquino, B 19; many more]
- Time domain formulation [Allix, Feissel, Nguyen 05; Allix, Feissel 06] (spatially 1D), [Aquino, B 14]

Error in constitutive relation (ECR)

$$
\boxed{\mathcal{E}(\pmb{v},\pmb{\tau},\pmb{\mathcal{C}})=0} \iff \text{(elastic) constitutive eq. satisfied (in $\pmb{L}^2(\Omega)$)}
$$

• Hence, elastic equilibrium problem, e.g.

 $v = \overline{u}$ on S_u (compatibility) $-d\mathsf{iv}\,\boldsymbol{\tau} = \boldsymbol{f}$ in Ω , $\boldsymbol{\tau} \cdot \boldsymbol{n} = \bar{\boldsymbol{t}}$ on S_{T} (equilibrium) $\tau = \mathcal{C}: \varepsilon[v]$ in Ω (constitutive)

as ECR minimization (for given material):

$$
(\boldsymbol{u}, \boldsymbol{\sigma}) = \mathop{\arg\min}_{(\boldsymbol{v}, \boldsymbol{\tau}) \in \mathcal{C}(\bar{\boldsymbol{u}}) \times \mathcal{S}(\bar{\boldsymbol{t}}, \, \boldsymbol{f})} \mathcal{E}(\boldsymbol{v}, \boldsymbol{\tau}, \boldsymbol{\mathcal{C}})
$$

Typically:

$$
\mathsf{KA} = \{ \, v \in \mathbf{H}^1(\Omega), \, v \text{ satisfies (compatibility)} \, \} \\ \mathsf{SA} = \{ \, \tau \in \mathbf{H}_{\mathsf{div}}(\Omega), \, \, \tau = \tau^{\mathsf{s}} \text{ and satisfies (equilibrium)} \, \}
$$

• Combines potential and complementary energy minimizations:

$$
\mathcal{E}(\mathbf{v}, \tau, \mathcal{C}) = \mathcal{P}(\mathbf{v}, \mathcal{C}) + \mathcal{P}^{\star}(\tau, \mathcal{C})
$$

$$
\mathcal{P}(\mathbf{v}) = \frac{1}{2} \int_{\Omega} \varepsilon[\mathbf{v}] : \mathcal{C} : \varepsilon[\mathbf{v}] \, dV - \int_{\Omega} \rho \mathbf{f} \cdot \mathbf{v} \, dV - \int_{S_T} \bar{\mathbf{t}} \cdot \mathbf{v} \, dS
$$

$$
\mathcal{P}^{\star}(\tau) = \frac{1}{2} \int_{\Omega} \tau : \mathcal{C}^{-1} : \tau \, dV - \int_{S_u} [\tau \cdot \mathbf{n}] \cdot \bar{\mathbf{u}} \, dS_x
$$

Variational formulations, error estimation

This retrieves well-known uncoupled minimizations of potential and complementary energies:

 $u = \arg \min \mathcal{P}(v, \mathcal{C})$ $v \in \mathcal{C}(\bar{u})$ $\mathcal{P}(v, \mathcal{C})$ $\sigma = \arg \min \, \mathcal{P}^{\star}(\tau, \mathcal{C})$ $\tau \in \mathcal{S}(\bar{t}, f)$

(i) $\mathcal{E}(\mathbf{u}, \sigma, \mathcal{C}) = \mathcal{E}(\mathcal{C}) = 0$ indicates that C is consistent with kinematic and static data. Performing either minimization suffices.

 $\bullet\,$ E.g. $\bm{u}=\arg\min \mathcal{P}(\bm{v},\bm{\mathcal{C}})$ then $\bm{\sigma}=\bm{\mathcal{C}}\!:\!\bm{\varepsilon}[\bm{u}]$ $v \in \mathcal{C}(\bar{u})$

(ii) $\mathcal{E}_h(\boldsymbol{u}_h, \boldsymbol{\sigma}_h, \boldsymbol{C}) = E_h(\boldsymbol{C}) \geq 0$ allows to defini error indicators *additive w.r.t. finite elements*

• Original motivation for introducing the ECR concept

(iii) $\mathcal{E}(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\mathcal{C}})=\mathcal{E}(\boldsymbol{\mathcal{C}})>0$ indicates that $\boldsymbol{\mathcal{C}}$ is not consistent with kinematic and static data.

• E.g. material identification / imaging problem with incorrectly known constitutive properties.

Generalization to other constitutive models

• (elastic) ECR given in terms of free energy and conjugate potentials ψ, ψ^*

$$
\mathcal{E}(\boldsymbol{v}, \boldsymbol{\tau}, \boldsymbol{\mathcal{C}}) = \int_{\Omega} \left(\underbrace{\psi(\boldsymbol{\varepsilon}[\boldsymbol{v}]) + \psi^{\star}(\boldsymbol{\tau}) - \boldsymbol{\tau} : \boldsymbol{\varepsilon}[\boldsymbol{v}]}_{\text{Legendre-Fenchel gap, } \geq 0} \right) dV
$$

$$
\psi(\varepsilon):=\tfrac{1}{2}\varepsilon\!:\!{\mathcal C}\!:\! \varepsilon,\quad \psi^\star(\tau):=\tfrac{1}{2}\tau\!:\!{\mathcal C}^{-1}\!:\! \tau.
$$

• More generally (small-strain nonlinear elasticity), same definition of $\mathcal{E}(v, \tau, \mathcal{C})$ if $\triangleright \psi$: convex free energy density with $\psi \geq 0$ and $\psi(0) = 0$; $\triangleright \psi^{\star}(\boldsymbol{\tau})$: (convex) conjugate potential $\psi^\star(\boldsymbol{\tau}) := \sup_{\boldsymbol{\varepsilon}} \big(\boldsymbol{\tau}\!:\!\boldsymbol{\varepsilon}-\psi(\boldsymbol{\varepsilon})\big)$

• Further generalization: generalized standard materials (GSMs) [Halphen, Nguyen 75; Germain, Nguyen, Suquet 83], in terms of free energy ψ and dissipation φ potentials: $\bm{\tau} = \bm{\tau}^{\sf rev} + \bm{\tau}^{\sf irr} = \partial_\varepsilon \psi(\bm{\varepsilon},\bm{\alpha}) + \partial_{\dot{\varepsilon}} \varphi(\dot{\bm{\varepsilon}},\dot{\bm{\alpha}}), \qquad \bm{A} = -\partial_\alpha \psi(\bm{\varepsilon},\bm{\alpha}) = \partial_{\dot{\alpha}} \varphi(\dot{\bm{\varepsilon}},\dot{\bm{\alpha}})$ (α) : internal variables, A: conjugate thermodynamic forces). ECR functionals then defined in terms of Legendre-Fenchel gaps

$$
\begin{aligned} &\psi(\varepsilon,\alpha)+\psi^\star(\tau^{\text{rev}},A)-\tau^{\text{rev}}\!:\varepsilon+A\!:\alpha\geq 0,\\ &\varphi(\dot{\varepsilon},\dot{\alpha})+\varphi^\star(\tau^{\text{irr}},A)-\tau^{\text{irr}}\!:\dot{\varepsilon}-A\!:\dot{\alpha}\geq 0. \end{aligned}
$$

ECR functionals may be defined (using Legendre-Fenchel gaps) for all GSMs.

ECR-based material identification

• Minimization of pure ECR:

$$
\mathcal{C} = \underset{\mathcal{B} \in \mathcal{Q}}{\arg \min} \left\{ \ \underset{\mathbf{v} \in \mathsf{KA}, \boldsymbol{\tau} \in \mathsf{SA}}{\min} \mathcal{E}(\mathbf{v}, \boldsymbol{\tau}, \boldsymbol{\mathcal{B}}) \right\}
$$

KA $=\left\{\textbf{\textit{v}}\in\textbf{\textit{H}}^{1}(\Omega),\textbf{\textit{v}}$ verifies all kinematic constraints and data $\right\}$ $\mathsf{SA} = \big\{ \boldsymbol{\tau} \! \in \! \boldsymbol{H}_{\mathsf{div}}(\Omega), \ \boldsymbol{\tau} \! = \! \boldsymbol{\tau}^{\mathsf{s}}$ and verifies all balance constraints

However, exact imposition of noisy data usually inadvisable.

• Minimization of modified ECR (MECR):

$$
\Lambda_{\kappa}(v, \tau, \mathcal{C}) := \mathcal{E}(v, \tau, \mathcal{C}) + \kappa \mathcal{D}(u - u_{\text{obs}})
$$
\n
$$
\mathcal{E} : \text{ original ECR} \qquad \mathcal{D} : \text{ quadratic} > 0 \text{ e.g. } \mathcal{D}(w) = \frac{1}{2} \mathcal{E}(w, \tau, \mathcal{C})
$$

- $\mathcal{E}:$ original ECR, $\mathcal{D}:$ quadratic ≥ 0 , e.g. $\mathcal{D}(w) = \frac{1}{2}$ $\int_{\Omega^m}|{\bm w}|^2\ {\rm d}V.$ \triangleright Enforces kinematic data via penalization (so data not embedded in KA space)
- \triangleright κ : tunable penalty (or coupling) parameter, akin to regularization (see later)

• Reduced MECR functional:

 $(u, \sigma) := \argmin_{v \in \text{KA}, \tau \in \text{SA}} \Lambda_{\kappa}(v, \tau, \mathcal{C}), \qquad \tilde{\Lambda}_{\kappa}(\mathcal{C}) := \Lambda_{\kappa}(u, \sigma, \mathcal{C})$ (PM)

▷ Quadratic partial minimization problem (see later), i.e. linear stationarity eqs.

- $\triangleright u = u[\mathcal{C}], \sigma = \sigma[\mathcal{C}]$ best compromise between (i) constitutive guess \mathcal{C} , (ii) measurements
- $\triangleright \tilde{\Lambda}_{\kappa}(\mathcal{C}) \neq 0$: residual MECR value reflecting incorrectly-known material.

Z

ECR-type functional for electrical impedance imaging

• Equations ($v:$ potential, $e:$ electric field, $q:$ current):

 $div g(x) = 0,$ $q(x) = a(x)e(x),$ $e(x) = -\nabla v(x)$

• ECR-type functional for N experiments with data \bar{v} for v and \bar{q} for q.n on $\partial\Omega$:

$$
\mathcal{E}(a, v_1, \dots, v_N, \mathbf{q}_1, \dots, \mathbf{q}_N) = \sum_{i=1}^N \int_{\Omega} \|a^{1/2} \nabla v + a^{-1/2} \mathbf{q}\|^2 dV
$$

Note:

$$
||a^{1/2}\nabla v + a^{-1/2}q||^2 = \frac{1}{a}|q + a\nabla v||^2 = \frac{1}{a}|q - ae||^2
$$

(a) "true" σ; reconstructions (b) no data noise.

Kohn R. V., Vogelius M., Comm. Pure Appl. Math. 40:745–777 (1987) Kohn R. V., McKenney A., Inverse Problems 6:389–414 (1990)

Energy (ECR-like) functional for ill-posed boundary value problems

Andrieux S., Baranger T., Ben Abda A., Inverse Problems 22:115–133 (2006)

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Framework

- Elastodynamic ECR-based reconstruction of heterogeneous elastic properties
- No prescribed boundary data:
	- \triangleright Well-posed forward problem a priori unclear (in contrast to usual inversion sitiations);
- This talk (based on [Aquino, B; SIAP (2019)]): internal kinematical data only
	- \triangleright (possibly overdetermined) boundary measurements may also be accounted for
	- ▷ Cases with well-posed BCs covered as special cases

 $\partial Ω = Γ$ (BC unknown)

Balance (SA): $\big(\boldsymbol{\sigma},\boldsymbol{\varepsilon}[\boldsymbol{w}]\big)_{\Omega} - \omega^2\big(\rho\boldsymbol{u},\boldsymbol{w}\big)_{\Omega} = \mathcal{F}(\boldsymbol{w}) \quad \text{for all } \boldsymbol{w} \in \mathcal{W} \!:=\! \boldsymbol{H}^1_0(\Omega),$ Kinematic compatibility (KA): (Ω), $\varepsilon[\boldsymbol{u}] = \frac{1}{2}(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^{\mathsf{T}})$ in Ω , Constitutive (linear elastic): $\sigma = \mathcal{C}: \varepsilon[u]$ in Ω .

Modified ECR (MECR) functional

MECR functional:

$$
\Lambda_{\kappa}(\boldsymbol{u},\boldsymbol{\sigma},\mathcal{C}):=\mathcal{E}(\boldsymbol{u},\boldsymbol{\sigma},\mathcal{C})+\kappa\mathcal{D}(\boldsymbol{u}-\boldsymbol{u}_{\mathrm{obs}})
$$

$$
\mathcal{E}(\boldsymbol{u},\boldsymbol{\sigma},\mathcal{C}):=\frac{1}{2}\int_{\Omega}(\boldsymbol{\sigma}-\mathcal{C}\!:\!\varepsilon[\boldsymbol{u}])\!:\!\mathcal{C}^{-1}\!:(\boldsymbol{\sigma}-\mathcal{C}\!:\!\varepsilon[\boldsymbol{u}])\;\mathrm{d}V
$$

$$
\mathcal{D}:\text{ quadratic}>0,\text{ e.g. }\mathcal{D}(\boldsymbol{w})=\frac{1}{2}\int_{\Omega^m}|\boldsymbol{w}|^2\;\mathrm{d}V
$$

- \triangleright Enforces kinematic data via penalization (so data not embedded in KA space)
- \triangleright κ : tunable penalty (or coupling) parameter, akin to regularization (see later)

Reduced MECR:

$$
(\boldsymbol{u},\boldsymbol{\sigma}):=\underset{\boldsymbol{v}\in\mathsf{KA},\boldsymbol{\tau}\in\mathsf{SA}}{\arg\min}\Lambda_{\kappa}(\boldsymbol{v},\boldsymbol{\tau},\boldsymbol{\mathcal{C}}),\qquad\tilde{\Lambda}_{\kappa}(\boldsymbol{\mathcal{C}}):=\Lambda_{\kappa}(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\mathcal{C}})
$$
\n(PM)

- ▷ Quadratic minimization problem (see later), i.e. linear stationarity eqs.
- $\triangleright u, \sigma$ best compromise between (i) constitutive guess C, (ii) measurements
- $\triangleright \tilde{\Lambda}_{\kappa}(\mathcal{C}) \neq 0$: residual MECR value reflecting incorrectly-known material.

Constitutive identification problem

Full-space approach:

$$
(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\mathcal{C}}):=\argmin_{\boldsymbol{v}\in\mathcal{U},\,\boldsymbol{\tau}\in\mathcal{S}(\boldsymbol{v}),\,\boldsymbol{\mathcal{C}}\in\mathcal{Q}}\Lambda_{\kappa}(\boldsymbol{v},\boldsymbol{\tau},\boldsymbol{\mathcal{C}}).
$$

Reduced-space approach: based on the reduced MECR:

 $(\boldsymbol{u}, \boldsymbol{\sigma}) := \arg \min \quad \Lambda_{\kappa}(\boldsymbol{v}, \boldsymbol{\tau}, \boldsymbol{\mathcal{C}}), \qquad \tilde{\Lambda}_{\kappa}(\boldsymbol{\mathcal{C}}) := \Lambda_{\kappa}(\boldsymbol{u}[\boldsymbol{\mathcal{C}}], \boldsymbol{\sigma}[\boldsymbol{\mathcal{C}}], \boldsymbol{\mathcal{C}})$ (PM) $v \in \mathcal{U}, \tau \in \mathcal{S}(v)$

(at least) two approaches for the constitutive identification problem:

1. Minimize $\tilde{\Lambda}_{\kappa}(\mathcal{C})$ (e.g. using CG, BFGS...)

Each evaluation of $\tilde{\Lambda}_{\kappa}(\mathcal{C}), \tilde{\Lambda}_{\kappa}'(\mathcal{C})$ needs to solve (PM).

- 2. Minimize $\Lambda_{\kappa}(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\mathcal{C}})$ via alternate directions
	- Field update (global) via (PM), C fixed: u, σ
	- Constitutive update (local, often closed-form)

$$
\boldsymbol{\mathcal{C}}^\star:=\underset{\boldsymbol{\mathcal{C}}\in\mathcal{Q}}{\arg\min}\,\tilde{\Lambda}_\kappa\left(\boldsymbol{\mathcal{C}}\right)
$$

$$
\boldsymbol{\mathcal{C}}^\star:=\argmin_{\boldsymbol{\mathcal{C}}\in\mathcal{Q}}\Lambda_{\kappa}(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\mathcal{C}})
$$

Problem (PM) plays a key role.

Stationarity equations

 $\sf Lagrangian$ (incorporating interior dynamical balance constraint with multiplier $\bm{w}\in \bm{H}_0^1(\Omega)$):

$$
\mathcal{L}(\boldsymbol{u}, \boldsymbol{\sigma}, \boldsymbol{w}, \mathcal{C}):=\mathcal{E}(\boldsymbol{u}, \boldsymbol{\sigma}, \mathcal{C})+\kappa \mathcal{D}(\boldsymbol{u}-\boldsymbol{u}_{\text{obs}})+\Big\{\big(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}[\boldsymbol{w}]\big)_{\Omega}-\omega^2\big(\rho \boldsymbol{u}, \boldsymbol{w}\big)_{\Omega}-\mathcal{F}(\boldsymbol{w})\Big\}, \\ \boldsymbol{w}\in \boldsymbol{H}^1_0(\Omega)
$$

First-order optimality conditions:

$$
\partial_{\mathbf{u}} \mathcal{L} = 0, \quad \partial_{\sigma} \mathcal{L} = 0, \quad \partial_{\mathbf{w}} \mathcal{L} = 0, \qquad \partial_{\mathcal{C}} \mathcal{L} = 0 \quad \partial_{\mathbf{u}} \mathcal{L} = 0, \quad \partial_{\sigma} \mathcal{L} = 0, \quad \partial_{\mathbf{w}} \mathcal{L} = 0, \qquad \partial_{\mathcal{C}} \mathcal{L} = 0
$$

(i) Partial minimization of $(u, \sigma) \mapsto \Lambda_{\kappa}(u, \sigma, \mathcal{C}) := \mathcal{E}(u, \sigma, \mathcal{C}) + \kappa \mathcal{D}(u-u_{\text{obs}}):$

$$
\sigma = \mathcal{C} : \varepsilon[u - w] , \qquad \begin{array}{l} \mathcal{A}(w, \widetilde{w}, \mathcal{C}) + \mathcal{B}(u, \widetilde{w}, \mathcal{C}) = \mathcal{F}(\widetilde{w}) & \text{for all } \widetilde{w} \in \mathcal{W} \\ \mathcal{B}(\widetilde{u}, w, \mathcal{C}) - \kappa \mathcal{D}(u, \widetilde{u}) = -\kappa \mathcal{D}(u_{\text{obs}}, \widetilde{u}) & \text{for all } \widetilde{u} \in \mathcal{U} \end{array}
$$

 $\mathcal{B}(\cdot,\cdot,\bm{\mathcal{C}}):=\mathcal{A}(\cdot,\cdot,\bm{\mathcal{C}})-\omega^2\mathcal{M}(\cdot,\cdot)$: dynamical stiffness bilinear form

(i) Partial minimization of $(u, \sigma) \mapsto \Lambda_{\kappa}(u, \sigma, \mathcal{C}) := \mathcal{E}(u, \sigma, \mathcal{C}) + \kappa \mathcal{D}(u-u_{\text{obs}}):$

$$
\sigma = \mathcal{C} : \varepsilon[u - w] , \qquad \begin{array}{l} \mathcal{A}(w, \widetilde{w}, \mathcal{C}) + \mathcal{B}(u, \widetilde{w}, \mathcal{C}) = \mathcal{F}(\widetilde{w}) & \text{for all } \widetilde{w} \in \mathcal{W} \\ \mathcal{B}(\widetilde{u}, w, \mathcal{C}) - \kappa \mathcal{D}(u, \widetilde{u}) = -\kappa \mathcal{D}(u_{\text{obs}}, \widetilde{u}) & \text{for all } \widetilde{u} \in \mathcal{U} \end{array}
$$

 $\mathcal{B}(\cdot,\cdot,\bm{\mathcal{C}}):=\mathcal{A}(\cdot,\cdot,\bm{\mathcal{C}})-\omega^2\mathcal{M}(\cdot,\cdot)$: dynamical stiffness bilinear form

(ii) Nonlinear stationarity equation on \mathcal{C} :

[Time-harmonic elastodynamics](#page-10-0)

Well-posedness of stationarity problem (finite-dimensional case)

• Coupled stationarity problem (replaces forward $+$ adjoint):

 $A(\mathbf{w}, \widetilde{\mathbf{w}}, \mathbf{C}) + B(\mathbf{u}, \widetilde{\mathbf{w}}, \mathbf{C}) = \mathcal{F}(\widetilde{\mathbf{w}})$ for all $\widetilde{\mathbf{w}} \in \mathcal{W}$ $\mathcal{B}(\tilde{\boldsymbol{u}}, \boldsymbol{w}, \boldsymbol{C}) - \kappa \mathcal{D}(\boldsymbol{u}, \tilde{\boldsymbol{u}}) = -\kappa \mathcal{D}(\boldsymbol{u}_{obs}, \tilde{\boldsymbol{u}})$ for all $\tilde{\boldsymbol{u}} \in \mathcal{U}$

- Let $\dim(\mathcal{U}) = n$, $\dim(\mathcal{W}) = m \leq n$. $A: \mathcal{W} \times \mathcal{W} \to \mathbb{R}$ \longrightarrow $A \in \mathbb{R}^{m \times m}$ $\mathcal{B} = \mathcal{A} - \omega^2 \mathcal{M}: \mathcal{U} \times \mathcal{W} \rightarrow \mathbb{R} \quad \longrightarrow \bm{B} \in \mathbb{R}^{m \times n}$ $\mathcal{D}: \mathcal{U} \times \mathcal{U} \to \mathbb{R}$ \longrightarrow $\mathbf{D} \in \mathbb{R}^{n \times n}$
- Discretized stationarity problem (BC setup such that \vec{A} invertible):

 $\begin{bmatrix} A & B \end{bmatrix}$ $\bm{B}^{\mathsf{T}} = -\kappa \bm{D}$ \mid \int w u $=\begin{cases} F \end{cases}$ $\kappa\bm{Du}^m$ ¹

• For any (u, w) solving the homogeneous system:

 $\boldsymbol{u}^{\mathsf{T}}\boldsymbol{B}^{\mathsf{T}}\boldsymbol{A}^{-1}\boldsymbol{B}\boldsymbol{u}+\kappa\boldsymbol{u}^{\mathsf{T}}\boldsymbol{D}\boldsymbol{u}=0$

Discrete stationarity system therefore well-posed if $N(B) \cap N(D) = \{0\}$

• Interpretation: available data must (more than) compensate lack of information on BCs

Well-posedness of stationarity problem (continuous case)

• Let $\mathcal{H} := \{ \boldsymbol{u} \in \mathcal{U}, \mid \mathcal{B}(\boldsymbol{u}, \widetilde{\boldsymbol{w}}, \mathcal{C}) = 0 \text{ for all } \widetilde{\boldsymbol{w}} \in \mathcal{W} \}$ underdetermined BCs on u (recall $W \subset U$)

Theorem (W. Aquino, MB, 2019):

Assume D coercive on $H \times H$ (i.e. data compensates insufficient BC information). The two-field stationarity problem

 $\mathcal{A}(\boldsymbol{w}, \widetilde{\boldsymbol{w}}, \mathcal{C}) + \mathcal{B}(\boldsymbol{u}, \widetilde{\boldsymbol{w}}, \mathcal{C}) = \mathcal{F}(\widetilde{\boldsymbol{w}})$ for all $\widetilde{\boldsymbol{w}} \in \mathcal{W}$
 $\mathcal{B}(\widetilde{\boldsymbol{u}}, \boldsymbol{w}, \mathcal{C}) - \kappa \mathcal{D}(\boldsymbol{u}, \widetilde{\boldsymbol{u}}) = -\kappa \mathcal{D}(\boldsymbol{u}_{\mathrm{obs}}, \widetilde{\boldsymbol{u}})$ for all $\widetilde{\boldsymbol{u}} \in \$

 $\mathcal{B}(\widetilde{\boldsymbol{u}},\boldsymbol{w},\boldsymbol{\mathcal{C}})-\kappa\mathcal{D}(\boldsymbol{u},\widetilde{\boldsymbol{u}})=-\kappa\mathcal{D}(\boldsymbol{u}_{\rm obs},\widetilde{\boldsymbol{u}})$

has a unique solution $(u, w) \in \mathcal{U} \times \mathcal{W}$, which is continuous in \mathcal{F}, u_{obs}

Proof method: Treat stationarity pb. as perturbed mixed problem [Boffi, Brezzi, Fortin 13].

Highlights: Stationarity problem is well-posed if sufficient full-field data available

- holds for all frequencies
- holds for (almost) all cases of BCs (including underdetermined BCs)
- $\bullet\,$ includes well-posed BC case, for which $\mathcal{U}=\mathcal{W}=\left\{\,\bm{u}\in \bm{H}^1(\Omega),\,\bm{u}=\bm{0}\,\,\text{on}\,\,\Gamma_{\textsf{D}}\,\right\}$ (say)

Shortcoming: Assumed coercivity of D on $\mathcal{H} \times \mathcal{H}$ in H^1 -norm.

Comparison with minimization of measurement misfit

- Conventional PDE-constrained constitutive identification: relation $\sigma = \mathcal{C}:\varepsilon[u]$ enforced.
- Lagrangian:

 $\mathcal{L}(\bm{u},\bm{w},\bm{\mathcal{C}}) := \mathcal{D}(\bm{u}-\bm{u}_{\text{obs}}) + \Big\{\big(\bm{\mathcal{C}}\!:\!\bm{\varepsilon}[\bm{u}], \bm{\varepsilon}[\bm{w}]\big)_{\Omega} - \omega^2 \big(\rho\bm{u},\bm{w}\big)_{\Omega} - \mathcal{F}(\bm{w})\Big\}, \quad \bm{w}\in \bm{H}_0^1(\Omega)$

• First-order optimality conditions:

 $\partial_{\alpha} \mathcal{L} = 0, \qquad \partial_{\alpha} \mathcal{L} = 0, \qquad \partial_{\alpha} \mathcal{L} = 0$

Forward and adjoint problems (coupled if $W \neq U$):

 $\mathcal{B}(\boldsymbol{u}, \widetilde{\boldsymbol{w}}, \mathcal{C}) = \mathcal{F}(\widetilde{\boldsymbol{w}})$ for all $\widetilde{\boldsymbol{w}} \in \mathcal{W}$ $\mathcal{B}(\widetilde{\boldsymbol{u}}, \boldsymbol{w}, \mathcal{C}) - \mathcal{D}(\boldsymbol{u}, \widetilde{\boldsymbol{u}}) = -\mathcal{D}(\boldsymbol{u}_{\text{obs}}, \widetilde{\boldsymbol{u}})$ for all $\widetilde{\boldsymbol{u}} \in \mathcal{U}$

Magnetic resonance elastography (S. Kurtz et al., Montpellier U. / Sherbrooke U.)

Coupled forward-adjoint implemented (for freq. domain elastodynamic sensing using 3D internal kinematic data) within a multizone approach

S. Kurtz, PhD 2023

Hessian of reduced MECR functional

- Consider reduced MECR functional $\tilde{\Lambda}_{\kappa}(\mathcal{C}) := \Lambda_{\kappa}(u, \sigma, \mathcal{C})$
- Expression of Hessian $\tilde{\Lambda}''_\kappa(\mathcal{C})$ established in terms of $\bm u_{\mathcal{C}}, \bm w_{\mathcal{C}}$ and $\bm u'_{\mathcal{C}}, \bm w'_{\mathcal{C}}$ (not shown)
- Large- κ expansion of stationarity solution (suitable if data noise low enough):

 $(\mathbf{u}, \mathbf{w}_{\mathcal{C}}) = (\mathbf{u}_0, \mathbf{w}_0) + \kappa^{-1}(\mathbf{u}_1, \mathbf{w}_1) + \dots$ (E)

with $(\mathbf{u}_{\ell}, \mathbf{w}_{\ell})$ $(\ell = 0, 1, 2, ...)$ defined as solutions of two-field problems.

• Insert (E) in $\tilde{\Lambda}_{\kappa}''(\mathcal{C})$ gives

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Theorem (MB, W. Aquino, 2019)
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For any \hat{\mathcal{C}} such that supp(\hat{\mathcal{C}}) \subset \Omega^m:
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$$
\tilde{\Lambda}_{\kappa}''(\mathcal{C})[\hat{\mathcal{C}}] = \tilde{\Lambda}_{0}''(\mathcal{C})[\hat{\mathcal{C}}] + \kappa^{-1} \tilde{\Lambda}_{1}''(\mathcal{C})[\hat{\mathcal{C}}] + o(\kappa^{-1})
$$

where $\tilde{\Lambda}_0''(\mathcal{C})[\hat{\mathcal{C}}]\geq 0$, $\tilde{\Lambda}_1''(\mathcal{C})[\hat{\mathcal{C}}]$ sign-indefinite

- \bullet $\tilde{\Lambda}''_\kappa$ is positive, i.e. $\tilde{\Lambda}_\kappa$ is "asymptotically convex", in the $\kappa\to\infty$ limit if $\mathsf{supp}(\hat{\bm{\mathcal{C}}})\subset\Omega^m$
- No such result available for L^2 minimization, even with complete internal data

Hessian of MECR functional

 $\Omega = (0, 1), -(E u')' - (2\pi f)^2 u = b, \quad u(0) = u(1) = 0, \qquad E = \chi_{[0,1/2]} E_1 + \chi_{[1/2,1]} E_2$

MECR-based alternate-direction reconstruction algorithm

 $\partial_{\mathcal{C}}\mathcal{L}=0$ \implies updating equations for the moduli.

- Assume unknown bulk and shear moduli B_E , G_E over element (groupings) E.
- Alternating direction minimization:
	- ⊳ At iteration q , available estimates G^{q-1} and B^{q-1} of moduli.
	- \triangleright Obtain u^q and w^q by solving the coupled systems of equations
	- \triangleright Update the moduli in each element or subdomain as

$$
B^q = \frac{\|s_k^q\|_{E,2}}{\|e_k^q\|_{E,2}}, \qquad 2G^q = \frac{\|s_k^q\|_{E,2}}{\|e_k^q\|_{E,2}}
$$

where $e_k(s_k)$: volumetric strain (stress) and $e_k(s_k)$: deviatoric strain (stress) associated with forward solution u and stress $\sigma = \mathcal{C}: \varepsilon[u-w]$.

- Correct updates B^q, G^q for possible violation of admissibility bounds.
- Morozov discrepancy criterion, if used: adjust κ to measurement noise δ through enforcement of $D(\kappa) = \delta^2$ (outer loop)

Morozov discrepancy criterion

- MECR functional: $\Lambda_{\kappa}(X, w; \kappa) := \mathcal{E}(X, w) + \kappa \mathcal{D}(X)$ with $X := (u, \sigma, \mathcal{C})$
- Set $E(\kappa) := \mathcal{E}(\mathbf{X}_{\kappa}, \mathbf{w}_{\kappa}), D(\kappa) := \mathcal{D}(\mathbf{X}_{\kappa})$ with $(X_{\kappa}, w_{\kappa}) := \arg \min_{\mathbf{X},w} \Lambda_{\kappa}(\mathbf{X},w;\kappa)$

Morozov discrepancy criterion: Seek \bm{X}_κ, κ such that $D(\kappa) = \delta^2$ (δ : data noise)

Lemma: (i) $\kappa \mapsto E(\kappa)$ is increasing; (ii) $\kappa \mapsto D(\kappa)$ is decreasing.

Consequently:

If $D(0) > \delta^2$, there exists κ such that $D(\kappa) = \delta^2$ (fulfilling Morozov's criterion)

Morozov discrepancy criterion

Proof of lemma: (a) we have $L'(\kappa)=\big<\partial_{\bm{X}}\mathcal{L},\bm{X}'\big> + \big<\partial_{\bm{w}}\mathcal{L},\bm{w}'\big> + \partial_{\kappa}\mathcal{L} = D(\kappa)$ and also $L'(\kappa) = E'(\kappa) + \kappa D'(\kappa) + D(\kappa)$; therefore $|E'(\kappa) + \kappa D'(\kappa) = 0|$. (b) We have $0 = \mathsf{d}_{\kappa} \big(\big\langle \partial_{\bm{X}} \mathcal{L}, \bm{X}' \big\rangle + \big\langle \partial_{\bm{w}} \mathcal{L}, \bm{w}' \big\rangle \big) = \big(L'(\kappa) - D(\kappa) \big)'.$ Moreover: $0 = \mathsf{d}_\kappa \big\langle \partial_{\bm{w}} \mathcal{L}, \bm{w}' \big\rangle$ (constraint verified for any κ), $0 = \mathsf{d}_{\kappa} \big \langle \partial_{\boldsymbol{X}} \mathcal{L}, \boldsymbol{X}' \big \rangle$ (stationarity eqs. verified for any κ) $\mathcal{L} = \left\langle \partial^2_{\boldsymbol{X}\boldsymbol{X}} \mathcal{L} , (\boldsymbol{X}',\boldsymbol{X}') \right\rangle + \left\langle \partial^2_{\boldsymbol{X}\boldsymbol{w}} \mathcal{L} , (\boldsymbol{X}',\boldsymbol{w}') \right\rangle + \left\langle \partial_{\boldsymbol{X}} \mathcal{L} , \boldsymbol{X}'' \right\rangle + D'(\kappa)$

$$
=\big\langle \partial^2_{\boldsymbol{X}}{}_{\boldsymbol{X}}\mathcal{L},(\boldsymbol{X}',\boldsymbol{X}')\big\rangle+D'(\kappa)
$$

and $\big\langle \partial^2_{\boldsymbol{X}\boldsymbol{X}}\mathcal{L},(\boldsymbol{X}',\boldsymbol{X}')\big\rangle\geq 0.$ Therefore $\Big|\,D'(\kappa)\leq 0\,\Big|$ and, by (a), $\Big|\,E'(\kappa)\geq 0\,\Big|.$

Example (2D reconstruction with 2D data and unknown BCs)

[Time-harmonic elastodynamics](#page-10-0)

Example (2D reconstruction with 2D data): alternated dirs vs. BFGS

Example (2D reconstruction with 2D data): alternated dirs vs. BFGS

Example (2D reconstruction with 2D data): alternated dirs vs. BFGS

2D example (Experimental data)

[Time-harmonic elastodynamics](#page-10-0)

2D example (Experimental data): imaging of shear modulus

Aquino, Babaniyi, Bayat, Fatemi 2017

1. [Concept of error in constitutive equation](#page-1-0)

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Modified ECR functional (transient, time-discrete)

Presentation after [B, Aquino, Inverse Problems (2014)]

- Time-stepping, $t_k = k\Delta t$ $(0 \le k \le N)$
- $\{u, v, a, \sigma\} := \{(u_k, v_k, a_k, \sigma_k)_{0 \leq k \leq N}\}.$ time-discrete histories (displacement, velocity, acceleration, stress)
- Time-discrete MECR functional:

$$
\Lambda_\kappa(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\mathcal{C}}):=\mathcal{E}_N(\boldsymbol{u},\boldsymbol{\sigma},\boldsymbol{\mathcal{C}})+\kappa\mathcal{D}_N(\boldsymbol{u})\qquad\text{ with e.g.}\quad \mathcal{D}_N(\boldsymbol{u}):=\frac{1}{2}
$$

$$
\text{with e.g.} \quad \mathcal{D}_N(\boldsymbol{u}) := \frac{1}{2} \sum_{k=1}^N \big| \boldsymbol{u}_k - \boldsymbol{u}_{\text{obs},k} \big|^2
$$

- Treat as constraints (i) initial and current interior balance eqns (in weak form) (ii) Newmark (β, γ) update relations
- Minimization of Λ_k : requires stationarity of Lagrangian \mathcal{L} :

$$
\mathcal{L}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{a}, \boldsymbol{\sigma}, \ \bar{\boldsymbol{u}}, \bar{\boldsymbol{v}}, \bar{\boldsymbol{a}}, \ \boldsymbol{C}) := \Lambda_{\kappa}(\boldsymbol{u}, \boldsymbol{\sigma}, \boldsymbol{C}) \n+ \sum_{k=0}^{N} \left\{ \left\langle \sigma_{k}, \varepsilon[\bar{u}_{k}] \right\rangle + \left\langle \rho a_{k}, \bar{u}_{k} \right\rangle - \mathcal{F}_{k}(\bar{u}_{k}) \right\} \n+ \sum_{k=1}^{N} \left\{ \left\langle (\boldsymbol{u}_{k} - \boldsymbol{u}_{k-1} - \Delta t \boldsymbol{v}_{k-1} - \Delta t^{2} \left[(1 - \beta) \boldsymbol{a}_{k-1} + \beta \boldsymbol{a}_{k} \right]), \ \bar{\boldsymbol{a}}_{k} \right\rangle \n+ \left\langle (\boldsymbol{v}_{k} - \boldsymbol{v}_{k-1} - \Delta t \left[(1 - \gamma) \boldsymbol{a}_{k-1} + \gamma \boldsymbol{a}_{k} \right]), \ \bar{\boldsymbol{v}}_{k} \right\rangle \right\}
$$

- Treatment valid for (more-general) α -generalized schemes (not discussed here)
- [Allix, Feissel, Nguyen 2005]: MECR for transient 1D case

Stationarity problem

$$
\left(\mathsf{a}\right)\left[\left.\partial_{\boldsymbol{\sigma}_k}\mathcal{L}=\mathbf{0}\right.\right]
$$

(b)
$$
\partial_{\bar{u}_k} \mathcal{L} = 0
$$
, $\partial_{\bar{v}_k} \mathcal{L} = 0$, $\partial_{\bar{a}_k} \mathcal{L} = 0$

(c)
$$
\partial_{\boldsymbol{u}_k} \mathcal{L} = \boldsymbol{0}, \quad \partial_{\boldsymbol{v}_k} \mathcal{L} = \boldsymbol{0}, \quad \partial_{\boldsymbol{a}_k} = \boldsymbol{0}
$$

 $\implies \sigma_k = \mathcal{C} : \varepsilon[u_k - \bar{u}_k]$

- \implies forward problem for (u, v, a) RHS depends on $(\bar{u}, \bar{v}, \bar{a})$ – unusual! Newmark
- \implies backward problem for $(\bar{u}, \bar{v}, \bar{a})$ RHS depends on (u, v, a) – usual adjoint Newmark
- (d) $\partial_{\mathcal{C}}\mathcal{L} = 0$ = \Rightarrow Constitutive updating formulae

Newmark and adjoint Newmark obey same stability conditions.

Alternate-direction minimization

For each iteration of main minimization loop:

- partial minimization of $\Lambda_\kappa(u,\sigma,\mathcal C)$: solve (a,b,c) for $(u^\star,v^\star,a^\star),\ (\bar u^\star,\bar v^\star,\bar a^\star)$ coupled forward-backward problem;
- partial minimization of $\Lambda_{\kappa}(u^{\star}, \sigma^{\star}, {\cal C})$: solve (d) for ${\cal C}^{\star}$ (analytical pointwise updating formulas \implies easy)

Coupled forward-backward problem $(a,b,c) \implies$ major computational bottleneck

Coupled forward-backward stationarity problem

Coupled system of stationarity equations, in block form:

$$
\begin{bmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{B}^{\mathsf{T}} & -\kappa \mathbb{D} \end{bmatrix} \begin{Bmatrix} \mathbb{W} \\ \mathbb{U} \end{Bmatrix} = \begin{Bmatrix} \mathbb{F} \\ \kappa \mathbb{D} \mathbb{U}^m \end{Bmatrix} \;,
$$

where

- \bullet $\mathbb{U}^{\intercal}:=\{(\bm{u}_0^{\intercal},\bm{v}_0^{\intercal},\bm{a}_0^{\intercal}),\ldots,(\bm{u}_N^{\intercal},\bm{v}_N^{\intercal},\bm{a}_N^{\intercal})\}$ (kinematical history);
- $\bullet\,$ $\mathbb{W}^{\intercal}:=\{(\bar{\bm{u}}_{0}^{\intercal},\bar{\bm{v}}_{0}^{\intercal},\bar{\bm{a}}_{0}^{\intercal}),\ldots,(\bar{\bm{u}}_{N}^{\intercal},\bar{\bm{v}}_{N}^{\intercal},\bar{\bm{a}}_{N}^{\intercal})\}$ (multiplier history);
- \mathbb{F} : applied excitation:
- \mathbb{B} : Newmark integrator, such that $\mathbb{B} \mathbb{U} = \mathbb{G}$ forward dynamical analysis; $\mathbb{B}^{\mathsf{T}}\mathbb{W} = \mathbb{H}$: backward dynamical analysis;
- A: (sym. s.p.d.) coupling matrix, from ECR part of Λ_{κ} ;
- \mathbb{D} : (sym. s.p.d.) "mass matrix", from L^2 measurement residual part of Λ_{κ} .

Kinematical constraints: $u_k \in \mathcal{U}$, $\bar{u}_k \in \mathcal{W}$ for all k. Blocks $\mathbb B$, $\mathbb B^{\mathsf T}$ are square if $\mathcal U=\mathcal W$, i.e. $\Gamma_{\mathsf D}=\Gamma\operatorname{\backslash} \Gamma_{\mathsf N}$ Stationarity problem: circumventing the coupling bottleneck

$$
\begin{bmatrix} \mathbb{B} & -\mathbb{A} \\ \kappa \mathbb{D} & \mathbb{B}^{\mathsf{T}} \end{bmatrix} \begin{Bmatrix} \mathbb{U} \\ \mathbb{W} \end{Bmatrix} = \begin{Bmatrix} \mathbb{F} \\ \kappa \mathbb{D} \mathbb{U}^m \end{Bmatrix} ,
$$

Proposed remedy to coupling bottleneck: block-SOR iterative scheme:

$$
\begin{bmatrix} \mathbb{B} & 0 \\ \eta \kappa \mathbb{D} & \mathbb{B}^\mathsf{T} \end{bmatrix} \begin{Bmatrix} \mathbb{U}^{(i+1)} \\ \mathbb{W}^{(i+1)} \end{Bmatrix} = \begin{bmatrix} (1-\eta)\mathbb{B} & -\eta \mathbb{A} \\ 0 & (1-\eta)\mathbb{B}^\mathsf{T} \end{bmatrix} \begin{Bmatrix} \mathbb{U}^{(i)} \\ \mathbb{W}^{(i)} \end{Bmatrix} + \begin{Bmatrix} \eta \mathbb{F} \\ \eta \kappa \mathbb{D} \mathbb{U}^m \end{Bmatrix}.
$$

 $(0 < n < 2$: relaxation parameter)

Convergence of block SOR algorithm

• Block-SOR and Jacobi iteration matrices (U: stationarity solution):

$$
\begin{Bmatrix} \mathbb{U}^{(i+1)} - \mathbb{U}^{\star} \\ \mathbb{W}^{(i+1)} - \mathbb{W}^{\star} \end{Bmatrix} = \mathbb{R}_{\alpha} \begin{Bmatrix} \mathbb{U}^{(i)} - \mathbb{U}^{\star} \\ \mathbb{W}^{(i)} - \mathbb{W}^{\star} \end{Bmatrix} \quad (\alpha = \text{J}, \text{SOR})
$$

- SOR converges iff $\rho_{SOR} := \rho(\mathbb{R}_{SOR}) < 1$
- Eigenvalues λ of \mathbb{R}_{SOR} and μ of \mathbb{R}_1 (simpler to evaluate) linked [Varga 62]

Proposition (MB, A. Aquino, 2015)

Let $\eta_0:=2(1+\rho_{\sf J})^{-1}$. Then, $\rho_{\sf SOR}(\eta)<1$ for any $\eta\in]0,\eta_0[$. Moreover:

(a) $\min_{\eta \in]0, \eta_0[} \rho_{\text{SOR}}(\eta) = 1 - \eta_1$ with $\eta_1 = 2/(1 + (1 + \rho_1^2)^{1/2})$ (b) $\rho_J = O(\kappa^{1/2})$, and hence $\lim_{\kappa \to \infty} \eta_0 = 0$, $\lim_{\kappa \to \infty} \min_{\eta \in [0, \eta_0[} \rho_{\text{SOR}}(\eta)) = 1$

 κ large (suitable for accurate data) (i) narrows convergence interval $[0, \eta_0[$ (ii) increases block-SOR iteration count

2D example (block SOR assessment)

- Load: time-harmonic pressure on top side (duration 1s, freq. 1Hz); bottom side clamped
- $(B_1, G_1) = (3, 2); (B_2, G_2) = (6, 4)$
- Full-field measured displacement for 1s duration
- Time step: $\Delta t = 0.01s$
- Meshes: 13,122 nodes (reconstruction, regular mesh), 19,216 nodes (data generation)

Simulations by WA, using the Sierra/SDA code of SANDIA Natl. Labs.

3D example (synthetic data)

- Load: time-harmonic pressure on top and side faces (duration 1s, freq. 1Hz); bottom face clamped
- Full-field measured displacement for 1s duration
- Time step: $\Delta t = 0.01s$
- Meshes: 50,000 nodes (reconstruction, regular mesh), 75,000 nodes (data generation)
- 550,000 unknown moduli

3D example (Synthetic data)

- About 200 MECR iterations;
- At most 5 SOR iterations per MECE iteration

1. [Concept of error in constitutive equation](#page-1-0)

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Introduction

This part follows [B, Salasiya, Guzina; JMPS (2024)]

- Material characterization of lossy solids treated as linear viscoelastic: applications e.g.
	- ▷ Account for lossy biological media in elastography
	- \triangleright Geomechanics, geophysics (dissipation linked to e.g. hydrocarbon reservoir parameters)

Viscoelastic characterization of rock specimens undergoing carbonation, excited under ultrasonically plane stress condition.

- Use of interior data feasible: ultrasound, MRI, laser vibrometer in rock mechanics
- This work:
	- \triangleright Extension to linear viscoelasticity of elastodynamic MECR with missing BC info Focus on case with interior measurement and no BC information
	- ▷ Both transient and time-harmonic cases treated

This work, US side funded by Center on Geo-processes in Mineral Carbon Storage, US Dept. of Energy

Linear viscoelastic solid as a generalized standard material

• Standard generalized material format for linear viscoelasticity:

 $\boldsymbol{\sigma}[\boldsymbol{u}] = \boldsymbol{\sigma}^\mathrm{e}[\boldsymbol{u}] + \boldsymbol{\sigma}^\mathrm{v}[\boldsymbol{u}]$

 $\bm{\sigma}^{\rm e}[\bm{u}] = \partial_{\varepsilon} \psi, \qquad\quad \bm{\sigma}^{\rm v}[\bm{u}] = \partial_{\varepsilon} \varphi, \qquad\quad \bm{A}[\bm{u}] = -\partial_{\alpha} \psi = \partial_{\dot{\alpha}} \varphi.$

• Free-energy potential and dissipation potential of general form (must be convex)

 $\psi(\boldsymbol{\varepsilon},\boldsymbol{\alpha})=\frac{1}{2}\big(\boldsymbol{\varepsilon}\!:\!\boldsymbol{\mathcal{C}}_{\varepsilon}\!:\!\boldsymbol{\varepsilon}+2\boldsymbol{\varepsilon}\!:\!\boldsymbol{\mathcal{C}}_{\mathrm{m}}\!:\!\boldsymbol{\alpha}+\boldsymbol{\alpha}\!:\!\boldsymbol{\mathcal{C}}_{\alpha}\!:\!\boldsymbol{\alpha}\big),$ $\varphi(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\alpha}}) = \frac{1}{2} (\dot{\boldsymbol{\varepsilon}} \cdot \boldsymbol{\mathcal{D}}_{\varepsilon} \cdot \dot{\boldsymbol{\varepsilon}} + 2 \dot{\boldsymbol{\varepsilon}} \cdot \boldsymbol{\mathcal{D}}_{\mathrm{m}} \cdot \dot{\boldsymbol{\alpha}} + \dot{\boldsymbol{\alpha}} \cdot \boldsymbol{\mathcal{D}}_{\alpha} \cdot \dot{\boldsymbol{\alpha}}), \qquad \qquad \mathbf{p} = \boldsymbol{\mathcal{C}}_{\varepsilon}, \boldsymbol{\mathcal{C}}_{\alpha}, \boldsymbol{\mathcal{D}}_{\varepsilon} \dots$

 $\triangleright \alpha$: "viscoelastic strain" internal variable.

 \triangleright $\mathcal{C}_{\varepsilon}$, \mathcal{C}_{α} , $\mathcal{D}_{\varepsilon}$, \mathcal{D}_{α} : 4th order tensors (maj + min symm., define positive quadratic forms, \triangleright $\mathcal{C}_{\rm m}$, $\mathcal{D}_{\rm m}$: 4th order tensors (min. symm., maj. symm. for convenience), s.t. ψ , $\varphi > 0$.

• Viscoelastic strain

$$
\partial_{\alpha}\psi + \partial_{\dot{\alpha}}\varphi = \mathbf{0} \implies \left[\alpha[\mathbf{u}](t) = -\boldsymbol{\mathcal{D}}_{\alpha}^{-1}\!:\!\boldsymbol{\mathcal{D}}_{\mathbf{m}}\!:\!\boldsymbol{\varepsilon}(t) - \mathbf{F}[\widehat{\boldsymbol{\mathcal{C}}}\!:\!\boldsymbol{\varepsilon}](t)\right]
$$

$$
\widehat{\mathbf{C}} := \mathbf{C}_{\mathrm{m}} - \mathbf{C}_{\alpha} : \mathbf{\mathcal{D}}_{\alpha}^{-1} : \mathbf{\mathcal{D}}_{\mathrm{m}}, \qquad \mathbf{F}[\mathbf{s}](t) = \int_{0}^{t} \exp[-\mathbf{\mathcal{D}}_{\alpha}^{-1} : \mathbf{\mathcal{C}}_{\alpha}(t-\tau)]: \mathbf{\mathcal{D}}_{\alpha}^{-1} : \mathbf{s}(\tau) d\tau
$$

• Stress-strain relation:

$$
\boldsymbol{\sigma}[\boldsymbol{u}](t) = \boldsymbol{\mathcal{C}}_1 \!:\! \boldsymbol{\varepsilon}(t) + \boldsymbol{\mathcal{D}}_1 \!:\! \dot{\boldsymbol{\varepsilon}}(t) - \boldsymbol{\widehat{\mathcal{C}}}^\mathsf{T} \!:\! \boldsymbol{\mathsf{F}}[\boldsymbol{\widehat{\mathcal{C}}} \!:\! \boldsymbol{\varepsilon}](t)
$$

with instantaneous tensors

 $\mathcal{C}_1 = \mathcal{C}_{\varepsilon} - \mathcal{C}_{\text{m}} : \mathcal{C}_{\alpha}^{-1} : \mathcal{C}_{\text{m}} + \widehat{\mathcal{C}}^{\top} : \mathcal{C}_{\alpha}^{-1} : \widehat{\mathcal{C}}, \qquad \mathcal{D}_1 = \mathcal{D}_{\varepsilon} - \mathcal{D}_{\text{m}} : \mathcal{D}_{\alpha}^{-1} : \mathcal{D}_{\text{m}}$

Inverse problem

• Identify (homogeneous or heterogeneous) VE parameters $\mathbf{p} = \mathcal{C}_{\varepsilon}, \mathcal{C}_{\alpha}, \mathcal{D}_{\varepsilon} \dots$ from interior kinematic data $\boldsymbol{u}_{\text{obs}}(\boldsymbol{\cdot},t)$ or $\boldsymbol{u}_{\text{obs}}(\boldsymbol{\cdot},\omega)$

 $\partial Ω = Γ$ (BC unknown)

• This work: MECR-based PDE-constrained approach

 $\min_{u,\sigma,\mathbf{p}} \mathcal{E}(u,\sigma,\mathbf{p}) + \kappa \mathcal{D}_T(u-u_{\text{obs}})$ s.t. u KA, σ DA $\mathcal{D}_T(v) = \frac{1}{2}$

$$
\boldsymbol{v}) = \tfrac{1}{2} \int_0^T \mathcal{D}(\boldsymbol{v}(t)) \, \mathrm{d}t
$$

Conjugate potentials:

$$
\psi^{\star}(\sigma^{\rm e}, A) = \max_{\varepsilon, \alpha} [\sigma^{\rm e}; \varepsilon - A; \alpha - \psi(\varepsilon, \alpha)],
$$

$$
\varphi^{\star}(\sigma^{\rm v}, A) = \max_{\varepsilon, \dot{\alpha}} [\sigma^{\rm v}; \dot{\varepsilon} + A; \dot{\alpha} - \varphi(\dot{\varepsilon}, \dot{\alpha})].
$$

• Legendre-Fenchel gaps:

$$
\epsilon_{\psi}(\varepsilon, \alpha, \sigma^{\rm e}, A) := \psi(\varepsilon, \alpha) + \psi^{\star}(\sigma^{\rm e}, A) - \sigma^{\rm e} : \varepsilon + A : \alpha \geq 0, \epsilon_{\varphi}(\dot{\varepsilon}, \dot{\alpha}, \sigma^{\rm v}, A) := \varphi(\dot{\varepsilon}, \dot{\alpha}) + \varphi^{\star}(\sigma^{\rm v}, A) - \sigma^{\rm v} : \dot{\varepsilon} - A : \dot{\alpha} \geq 0.
$$

Chosen pointwise ECR: $e_{\text{ECR}}(\boldsymbol{x},t) = \epsilon_{\psi}(\boldsymbol{x},t) + T \epsilon_{\varphi}(\boldsymbol{x},t)$.

Example: standard linear solid

$$
\mathcal{C}_{\varepsilon} = -\mathcal{C}_{m} = \mathcal{C}_{1}, \qquad \mathcal{C}_{\alpha} = \mathcal{C}_{1} + \mathcal{C}_{2}, \qquad \mathcal{D}_{\alpha} = \mathcal{D}, \qquad \mathcal{D}_{\varepsilon} = \mathcal{D}_{m} = 0,
$$
\n
$$
\psi(\varepsilon, \alpha) = \frac{1}{2}(\varepsilon - \alpha) : \mathcal{C}_{1} : (\varepsilon - \alpha) + \frac{1}{2}\alpha : \mathcal{C}_{2} : \alpha, \qquad \varphi(\varepsilon, \dot{\alpha}) = \frac{1}{2}\dot{\alpha} : \mathcal{D} : \dot{\alpha},
$$
\n
$$
\psi^{*}(\sigma, A) = \frac{1}{2}(\sigma - A) : \mathcal{C}_{2}^{-1} : (\sigma - A) + \frac{1}{2}\sigma : \mathcal{C}_{1}^{-1} : \sigma, \qquad \varphi^{*}(A) = \frac{1}{2}A : \mathcal{D}^{-1} : A.
$$
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Pointwise Legendre-Fenchel gaps:

$$
e_{\psi} = \frac{1}{2} (\boldsymbol{\sigma} - \mathcal{C}_1 : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha})) : \mathcal{C}_1^{-1} : (\boldsymbol{\sigma} - \mathcal{C}_1 : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha})) + \frac{1}{2} (\boldsymbol{\sigma} - \boldsymbol{A} - \mathcal{C}_2 : \boldsymbol{\alpha}) : \mathcal{C}_2^{-1} : (\boldsymbol{\sigma} - \boldsymbol{A} - \mathcal{C}_2 : \boldsymbol{\alpha}))
$$

\n
$$
e_{\varphi} = \frac{1}{2} (\boldsymbol{A} - \boldsymbol{\mathcal{D}} : \dot{\boldsymbol{\alpha}}) : \boldsymbol{\mathcal{D}}^{-1} : (\boldsymbol{A} - \boldsymbol{\mathcal{D}} : \dot{\boldsymbol{\alpha}}).
$$

MECR-based minimization

• Displacement spaces:

$$
\mathcal{U}:=\mathcal{V},\qquad \mathcal{W}:=\big\{\,\textcolor{blue}{v\in\mathcal{V}},\,\textcolor{blue}{v=0}\,\,\text{on}\,\,\Gamma\,\big\}\subset\mathcal{U}
$$

- $\mathcal V$: energy space, e.g. $\mathcal V=H^1(\Omega\times[0,T];\mathbb R^d)$ (transient), $\mathcal V=H^1(\Omega;\mathbb R^d)$ (time-harmonic)
- Interior balance of linear momentum, weak form (interior equations only):

$$
\int_{\Omega}\int_0^T \big(\boldsymbol{\sigma}\!:\!\boldsymbol{\varepsilon}[\boldsymbol{w}]+\rho\ddot{\boldsymbol{u}}\!\cdot\!\boldsymbol{w}\big)\,\mathrm{d} t\,\mathrm{d} V=0\qquad\forall\,\boldsymbol{w}\in\mathcal{W}.
$$

 $\bullet\,$ Overall constitutive mismatch for given ${\bf p}$ (with ${\bf X}:=(\bm u,\bm \alpha,\bm \sigma^{\rm e},\bm \sigma^{\rm v},\bm A)$):

$$
\mathcal{E}(\mathbf{X}, \mathbf{p}) = \mathcal{E}^{\mathbf{e}}(\boldsymbol{\varepsilon}[\boldsymbol{u}], \boldsymbol{\alpha}, \boldsymbol{\sigma}^{\mathbf{e}}, \boldsymbol{A}, \mathbf{p}) + \mathcal{E}^{\mathbf{v}}(\dot{\boldsymbol{\varepsilon}}[\boldsymbol{u}], \dot{\boldsymbol{\alpha}}, \boldsymbol{\sigma}^{\mathbf{v}}, \boldsymbol{A}, \mathbf{p})],
$$

$$
\mathcal{E}^{\mathbf{e}} := \int_{\Omega} \int_{0}^{T} \epsilon_{\psi}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}, \boldsymbol{\sigma}^{\mathbf{e}}, \boldsymbol{A}, \mathbf{p}) \, \mathrm{d}t \, \mathrm{d}V, \qquad \mathcal{E}^{\mathbf{v}} := \int_{\Omega} \int_{0}^{T} T \epsilon_{\varphi}(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\alpha}}, \boldsymbol{\sigma}^{\mathbf{v}}, \boldsymbol{A}, \mathbf{p}) \, \mathrm{d}t \, \mathrm{d}V.
$$

• Modified ECR (MECR) functional:

$$
\Lambda_{\kappa}(\mathbf{X}, \mathbf{p}) := \mathcal{E}(\mathbf{X}, \mathbf{p}) + \frac{1}{2} \kappa \mathcal{D}_{\mathcal{T}}(\boldsymbol{u} - \boldsymbol{u}_{\text{obs}}, \boldsymbol{u} - \boldsymbol{u}_{\text{obs}}),
$$

• Find compromise p, X (constitutive equations vs. data reproduction): PDE-constrained minimization

$$
\min_{{\mathbf{X}}, {\mathbf{p}}} \Lambda_\kappa({\mathbf{X}}, {\mathbf{p}}) \qquad \text{subject to } {\bm{u}} \in \mathcal{U} \ \ \text{and} \ \ (\text{weak}) \ \text{balance eq.}\ .
$$

1st-order optimality conditions of MECR functional

 $\min_{\mathbf{w}} \Lambda_{\kappa}(\mathbf{X}, \mathbf{p})$ subject to $\boldsymbol{u} \in \mathcal{U}$ and (weak) balance eq. . X,p

• Lagrangian (Lagrange multiplier $w \in \mathcal{W}$):

$$
\mathcal{L}(\mathbf{X}, \mathbf{w}, \mathbf{p}) := \Lambda_{\kappa}(\mathbf{X}, \mathbf{p}) - \int_{\Omega} \int_{0}^{T} ((\boldsymbol{\sigma}^{\mathbf{e}} + \boldsymbol{\sigma}^{\mathbf{v}}) \cdot \boldsymbol{\varepsilon}[\mathbf{w}] + \rho \ddot{\mathbf{u}} \cdot \mathbf{w}) \, \mathrm{d}t \, \mathrm{d}V.
$$

- 1st-order optimality conditions: stress and internal variables:
	- (a) $\left\langle \partial_{\sigma^{\mathbf{e}}}\mathcal{L},\widehat{\sigma}^{\mathbf{e}} \right\rangle =0 \quad \forall \ \widehat{\sigma}^{\mathbf{e}},$ (c) $\left\langle \partial_{A}\mathcal{L},\widehat{A} \right\rangle =0 \quad \forall \ \widehat{A},$ (b) $\langle \partial_{\sigma} v \mathcal{L}, \hat{\sigma}^v \rangle = 0 \quad \forall \hat{\sigma}^v,$ (d) $\langle \partial_{\alpha} \mathcal{L}, \hat{\alpha} \rangle = 0 \quad \forall \hat{\alpha}.$

1st-order optimality conditions: kinematical variables:

- (a) $\left\langle \partial_w \mathcal{L}, \widehat{\bm{w}} \right\rangle = 0 \quad \forall \ \widehat{\bm{w}},$
- (b) $\langle \partial_u \mathcal{L}, \widehat{\mathbf{u}} \rangle = 0 \quad \forall \, \widehat{\mathbf{u}},$

1st-order optimality conditions: material parameters:

 $\langle \partial_{\mathbf{p}} \mathcal{L}, \widehat{\mathbf{p}} \rangle = 0 \quad \forall \, \widehat{\mathbf{p}}.$

1st-order optimality conditions: local equations

Local stationarity equations ($\varepsilon \equiv \varepsilon[u]$, $\eta \equiv \varepsilon[w]$)

(a)
$$
0 = \int_{\Omega} \int_0^T \left\{ \partial_{\sigma^e} \psi^{\star} - \varepsilon - \eta \right\} : \widehat{\sigma}^e \, dt \, dV \qquad \forall \widehat{\sigma}^e,
$$

(b)
$$
0 = \int_{\Omega} \int_0^T \left\{ T(\partial_{\sigma^{\mathrm{v}}} \varphi^{\star} - \dot{\varepsilon}) - \eta \right\} : \hat{\sigma}^{\mathrm{v}} \, \mathrm{d}t \, \mathrm{d}V \qquad \forall \hat{\sigma}^{\mathrm{v}},
$$

(c)
$$
0 = \int_{\Omega} \int_0^T \left\{ \partial_A \psi^* + \alpha + T \big(\partial_A \varphi^* - \dot{\alpha} \big) \right\} : \hat{A} dt dV \qquad \forall \hat{A},
$$

(d)
$$
0 = \int_{\Omega} \int_0^T \left\{ \big(\partial_\alpha \psi + A \big) : \hat{\alpha} + T \big(\partial_{\dot{\alpha}} \varphi - A \big) : \hat{\alpha} \right\} dt dV \qquad \forall \hat{\alpha}, \hat{\alpha}(\cdot, 0) = 0.
$$

Closed-form solution:

(a), (b), (c)
$$
\implies
$$

$$
\begin{cases} \sigma^{\rm e} = \mathcal{C}_{\varepsilon} : \varepsilon + \mathcal{C}_{\rm m} : \alpha + (\mathcal{C}_{\varepsilon}^{\rm s} + \mathcal{C}_{\rm m} : \mathcal{C}_{\alpha}^{-1} : \widehat{\mathcal{C}}) : \eta - \mathcal{C}_{\rm m} : \beta, \\ \sigma^{\rm v} = \mathcal{D}_{\rm m} : \dot{\alpha} + \mathcal{D}_{\varepsilon} : \dot{\varepsilon} + \frac{1}{T} \mathcal{D}_{\rm l} : \eta - \frac{1}{T} \mathcal{D}_{\rm m} : \beta, \\ A = \mathcal{D}_{\alpha} : \dot{\alpha} + \mathcal{D}_{\rm m} : \dot{\varepsilon} - \frac{1}{T} \mathcal{D}_{\alpha} : \beta, \end{cases}
$$

 $(\frac{1}{T}{\cal D}_{\alpha}+{\cal C}_{\alpha})\!:\!\beta={\cal D}_{\alpha}\!:\!\dot{\alpha}+{\cal D}_{\rm m}\!:\!\dot{\varepsilon}+{\cal C}_{\alpha}\!:\!\alpha+{\cal C}_{\rm m}\!:\!\varepsilon+\widehat{\cal C}\!:\!\eta.$

(d)
$$
\implies
$$
 0 = $\partial_{\alpha}\psi + A - T\partial_{t}(\partial_{\dot{\alpha}}\varphi - A),$ 0 = $(\partial_{\dot{\alpha}}\varphi - A)(T),$
\n \implies $\mathcal{D}_{\alpha}:\dot{\beta} - \mathcal{C}_{\alpha}:\beta + \hat{\mathcal{C}}:\eta = 0,$ $\beta(T) = 0$ using (a)-(c)
\n $\implies \boxed{\beta(t) = \mathsf{F}_{R}[\hat{\mathcal{C}}:\eta_{R}](t)}$ $(f_{R}(t) = f(T-t))$
\nM. Bonnet (POEMS, ENSTA)
\nError in constitutive relation for material identification

1st-order optimality conditions: local equations

(a), (b), (c)
$$
\Rightarrow \begin{bmatrix} \sigma^e = \mathcal{C}_{\varepsilon} : \varepsilon + \mathcal{C}_{\rm m} : \alpha + (\mathcal{C}_{\varepsilon}^S + \mathcal{C}_{\rm m} : \mathcal{C}_{\alpha}^{-1} : \widehat{\mathcal{C}}) : \eta - \mathcal{C}_{\rm m} : \beta, \\ \sigma^{\rm v} = \mathcal{D}_{\rm m} : \dot{\alpha} + \mathcal{D}_{\varepsilon} : \dot{\varepsilon} + \frac{1}{T} \mathcal{D}_{\rm l} : \eta - \frac{1}{T} \mathcal{D}_{\rm m} : \beta, \\ A = \mathcal{D}_{\alpha} : \dot{\alpha} + \mathcal{D}_{\rm m} : \dot{\varepsilon} - \frac{1}{T} \mathcal{D}_{\alpha} : \beta, \\ (\frac{1}{T} \mathcal{D}_{\alpha} + \mathcal{C}_{\alpha}) : \beta = \mathcal{D}_{\alpha} : \dot{\alpha} + \mathcal{D}_{\rm m} : \dot{\varepsilon} + \mathcal{C}_{\alpha} : \alpha + \mathcal{C}_{\rm m} : \varepsilon + \widehat{\mathcal{C}} : \eta. \end{bmatrix},
$$
(*)

(d)
$$
\implies
$$
 $\beta(t) = \mathbf{F}_{R}[\hat{\mathcal{C}} : \eta_{R}](t)$

- Use β in (\star) , to obtain $\boldsymbol{\alpha}(t) = \boldsymbol{\alpha}[\boldsymbol{u}](t) + \textbf{F}[\boldsymbol{\mathcal{D}}_{\alpha} \, \vdots \, (\frac{1}{T}\boldsymbol{\beta} + \boldsymbol{\beta})](t)$ Finally, evaluate $\sigma = \sigma^{\rm e} + \sigma^{\rm v}$ to find $\boldsymbol{\sigma}(t) = \boldsymbol{\sigma}[\boldsymbol{u}](t) + \boldsymbol{\mathcal{S}}_t[\boldsymbol{w}](t) \quad \boldsymbol{\mathcal{S}}_t[\boldsymbol{w}] = (\boldsymbol{\mathcal{C}}_1 + \frac{1}{T}\boldsymbol{\mathcal{D}}_1) : \boldsymbol{\eta} + \boldsymbol{\widehat{\mathcal{C}}}^\intercal : (\boldsymbol{\alpha} - \boldsymbol{\alpha}[\boldsymbol{u}] - \boldsymbol{\beta}).$
- Key property:

$$
\int_0^T \mathcal{S}_t[\boldsymbol{w}] : \boldsymbol{\eta} \, \mathrm{d} t = \int_0^T \left\{ \boldsymbol{\eta} : \left(\mathcal{C}_{\varepsilon}^{\mathsf{S}} + \frac{1}{T} \mathcal{D}_\mathsf{I} \right) : \boldsymbol{\eta} + \frac{1}{T} \boldsymbol{\beta} : \mathcal{D}_{\alpha} : \boldsymbol{\beta} + \dot{\boldsymbol{\beta}} : \mathcal{D}_{\alpha} : \mathcal{C}_{\alpha}^{-1} : \mathcal{D}_{\alpha} : \dot{\boldsymbol{\beta}} \right\} \mathrm{d} t \geqslant 0.
$$

Purely elastic case much simpler:

$$
\left|\right.\boldsymbol{\sigma}(t)=\boldsymbol{\sigma}[\boldsymbol{u}](t)+\boldsymbol{\sigma}[\boldsymbol{w}](t)=\boldsymbol{\mathcal{C}}_{\varepsilon}\!:\!\boldsymbol{\varepsilon}[\boldsymbol{u}+\boldsymbol{w}]\,\right|\;\text{sole local eqn.}
$$

1st-order optimality conditions: global equations

• A priori:

$$
\int_{\Omega} \int_{0}^{T} \left(\sigma : \varepsilon[\hat{w}] + \rho \hat{u} \cdot \hat{w} \right) dt dV = 0 \qquad \forall \hat{w} \in \mathcal{W}.
$$

$$
\int_{\Omega} \int_{0}^{T} \left\{ \left(\partial_{\varepsilon} \psi - \sigma^{\mathrm{e}} \right) : \varepsilon[\hat{u}] + T \left(\partial_{\varepsilon} \varphi - \sigma^{\mathrm{v}} \right) : \varepsilon[\hat{u}] - \rho w \cdot \hat{u} \right\} dt dV + \kappa \int_{0}^{T} \mathcal{D}(u - u_{\mathrm{obs}}, \hat{u}) dt = 0 \qquad \forall \hat{u} \in \mathcal{U}.
$$

• Use $\sigma = \sigma[u] + \mathcal{S}_{t}[w]$, integrate by parts in time, use results from local stationarity ends
and reciprocity identity $\int_{0}^{T} (\sigma[u] : \varepsilon[w] - \sigma_{\mathrm{R}}[w_{\mathrm{R}}] : \varepsilon[u]) dt = (\varepsilon[w] : \mathcal{D}_{\mathrm{I}} : \varepsilon[u]) \Big|_{0}^{T}.$
Obtain forward-backward (underdetermined / overdetermined) stationarity system for u, w :

$$
\int_{\Omega} \int_{0}^{T} (\sigma[u] : \varepsilon[\hat{w}] + \rho \ddot{u} \cdot \hat{w}) dt dV + \int_{\Omega} \int_{0}^{T} \mathcal{S}_{t}[w] : \varepsilon[\hat{w}] dt dV = 0 \qquad \forall \hat{w} \in \mathcal{W},
$$

$$
u(\cdot, 0) = \dot{u}(\cdot, 0) = 0 \qquad \text{in } \Omega,
$$

$$
\int_{\Omega} \int_{0}^{T} (\sigma_{\mathrm{R}}[w_{\mathrm{R}}] : \varepsilon[\hat{u}] + \rho \ddot{w} \cdot \hat{u}) dt dV - \kappa \int_{0}^{T} \mathcal{D}(u, \hat{u}) dt = -\kappa \int_{0}^{T} \mathcal{D}(u_{\mathrm{obs}}, \hat{u}) dt
$$

• Unique solvability for $(u, w) \in U \times W$ expected if (i) sufficient data u_{obs} , (ii) cnds. on \mathcal{D}_{τ} . (by analogy with time-harmonic elastic case [Aquino, B 19])

Ω

 $\forall \widehat{\mathbf{u}} \in \mathcal{U},$

 $w(\cdot, T) = \dot{w}(\cdot, T) = 0$ in Ω .

Some remarks

• If more-general boundary decomposition $\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_c$ (with possibly $|\Gamma_c| \neq 0$), use $\mathcal{U}:=\left\{\,\boldsymbol{v}\in\mathcal{V},\,\boldsymbol{v}\!=\!\boldsymbol{0} \,\,\textsf{on}\,\,\Gamma_{\mathsf{D}}\,\right\}, \qquad \mathcal{W}:=\left\{\,\boldsymbol{v}\in\mathcal{V},\,\boldsymbol{v}\!=\!\boldsymbol{0} \,\,\textsf{on}\,\,\Gamma_{\mathsf{D}}\cup\Gamma_{c}\,\right\}\subset\mathcal{U}.$

• For well-posed BCs, $|\Gamma_c| = 0$ and $W = U$.

If additional prescribed excitations, weak balance of linear momentum becomes

$$
\int_{\Omega}\int_0^T \big(\boldsymbol{\sigma}\!:\!\boldsymbol{\varepsilon}[\boldsymbol{w}]+\rho\ddot{\boldsymbol{u}}\!\cdot\!\boldsymbol{w}\big)\,\mathrm{d} t\,\mathrm{d} V=\mathcal{F}(\boldsymbol{w})\qquad\forall\,\boldsymbol{w}\in\mathcal{W},
$$

- Initial (final) rest assumed for simplicity for $u(w)$. How to adapt to cases with unknown initial values for u ?
- Weighted ECR of form $\mathcal{E} = \mathcal{E}^{\text{e}} + \gamma \mathcal{E}^{\text{v}}$ easy to implement (e.g. stronger focus on dissipation).

MECR formulation for the time-harmonic case

• Conventions: $T = 2\pi/\omega$ and

$$
\int_{\Omega} \int_0^T \mathbf{u} \cdot \mathbf{v} \, dV \, dt = \frac{\pi}{\omega} \int_{\Omega} \text{Re}(\mathbf{u} \cdot \overline{\mathbf{v}}) \, dV, \qquad \big\langle \partial_{\mathbf{x}} f, \widehat{\mathbf{x}} \big\rangle = \text{Re}\big\{ \big(\partial_{\mathbf{x}_R} f + \mathrm{i} \partial_{\mathbf{x}_I} f \big) \cdot \overline{\widehat{\mathbf{x}}} \big\}
$$

• Quadratic potentials become Hermitian forms, and

$$
\psi(\varepsilon,\alpha) = \frac{1}{2} \big(\varepsilon : \mathcal{C}_{\varepsilon} : \bar{\varepsilon} + \alpha : \mathcal{C}_{m} : \bar{\varepsilon} + \varepsilon : \mathcal{C}_{m} : \bar{\alpha} + \alpha : \mathcal{C}_{\alpha} : \bar{\alpha} \big),
$$

$$
\sigma^e[u] = \mathcal{C}_{\varepsilon} : \varepsilon + \mathcal{C}_{m} : \alpha, \qquad \sigma^v[u] = -i\omega(\mathcal{D}_{\varepsilon} : \varepsilon + \mathcal{D}_{m} : \alpha),
$$

$$
\varphi(\dot{\varepsilon}, \dot{\alpha}) = \omega^2 \varphi(\varepsilon, \alpha), \qquad \partial_{\dot{\alpha}} \varphi(\dot{\varepsilon}, \dot{\alpha}) = -i\omega \partial_{\alpha} \varphi(\varepsilon, \alpha)
$$

• Time-harmonic constitutive relation

 $\boldsymbol{\sigma}[\boldsymbol{u}] = (\boldsymbol{\sigma}^\mathrm{e} + \boldsymbol{\sigma}^\mathrm{v})[\boldsymbol{u}] = \boldsymbol{\mathcal{C}}(\omega)\!:\!\boldsymbol{\varepsilon},$ $\mathcal{C}(\omega) = (\mathcal{C}_{\varepsilon} - \mathrm{i} \omega \mathcal{D}_{\varepsilon}) - (\mathcal{C}_{\mathrm{m}} - \mathrm{i} \omega \mathcal{D}_{\mathrm{m}})$: $(\mathcal{C}_{\alpha} - \mathrm{i} \omega \mathcal{D}_{\alpha})^{-1}$: $(\mathcal{C}_{\mathrm{m}} - \mathrm{i} \omega \mathcal{D}_{\mathrm{m}})$

Stationarity system for the time-harmonic case

• Time-harmonic ECR functional:

$$
\mathcal{E}(\mathbf{X}, \mathbf{p}; \omega) := \int_{\Omega} \left\{ \epsilon_{\psi}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}, \boldsymbol{\sigma}^{\mathrm{e}}, \boldsymbol{A}, \mathbf{p}) + T \epsilon_{\varphi}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}, \boldsymbol{\sigma}^{\mathrm{v}}, \boldsymbol{A}, \mathbf{p}; \omega) \right\} dV,
$$

with Legendre-Fenchel gaps given by

 $\epsilon_\psi(\boldsymbol{\varepsilon},\boldsymbol{\alpha},\boldsymbol{\sigma}^\mathrm{e},\boldsymbol{A},\boldsymbol{\mathsf{p}}) := \psi(\boldsymbol{\varepsilon},\boldsymbol{\alpha},\boldsymbol{\mathsf{p}}) + \psi^\star(\boldsymbol{\sigma}^\mathrm{e},\boldsymbol{A},\boldsymbol{\mathsf{p}}) - \mathsf{Re}\big[\boldsymbol{\sigma}^\mathrm{e}\!:\!\bar{\boldsymbol{\varepsilon}}-\boldsymbol{A}\!:\!\bar{\boldsymbol{\alpha}}\big],$

 $\epsilon_\varphi(\boldsymbol{\varepsilon},\boldsymbol{\alpha},\boldsymbol{\sigma}^{\text{v}},\boldsymbol{A},\mathsf{p};\omega) := \omega^2\varphi(\boldsymbol{\varepsilon},\boldsymbol{\alpha},\mathsf{p}) + \varphi^\star(\boldsymbol{\sigma}^{\text{v}},\boldsymbol{A},\mathsf{p}) - \mathsf{Re}\big[\hspace{1pt}\mathrm{i}\omega(\boldsymbol{\sigma}^{\text{v}}\!:\!\bar{\boldsymbol{\varepsilon}}+\boldsymbol{A}\!:\!\bar{\boldsymbol{\alpha}})\big],$

• MECR functional:

$$
\Lambda_{\kappa}(\mathbf{X}, \mathbf{p}; \omega) := \mathcal{E}(\mathbf{X}, \mathbf{p}; \omega) + \frac{1}{2} \kappa \mathcal{D}(\mathbf{u} - \mathbf{u}_{\text{obs}}, \overline{\mathbf{u} - \mathbf{u}_{\text{obs}}}),
$$

• Lagrangian (with Lagrange multiplier $w \in \mathcal{W}$):

$$
\mathcal{L}(\mathbf{X}, \mathbf{w}, \mathbf{p}; \omega) := \Lambda_{\kappa}(\mathbf{X}, \mathbf{p}; \omega) - \text{Re} \Big\{ \int_{\Omega} \big((\boldsymbol{\sigma}^{\text{e}} + \boldsymbol{\sigma}^{\text{v}}) : \boldsymbol{\varepsilon}[\bar{\boldsymbol{w}}] - \rho \omega^2 \boldsymbol{u} \cdot \bar{\boldsymbol{w}} \big) \, \mathsf{d}V \Big\}.
$$

Local stationarity equations yield

 $\sigma = \mathcal{C}(\omega) : \epsilon + \mathcal{S}(\omega) : n$

where $\mathcal{S}(\omega)$ Hermitian positive definite:

 $\mathcal{S}(\omega) = \mathcal{C}_{\varepsilon}^{\mathsf{S}} + \frac{1}{T}\mathcal{D}_{\mathsf{I}} + \widehat{\mathcal{C}}^{\mathsf{T}} \cdot (\mathcal{C}_{\alpha} - \mathrm{i}\omega \mathcal{D}_{\alpha})^{-1} \cdot (\frac{1}{T}\mathcal{D}_{\alpha} + \omega^2 \mathcal{D}_{\alpha} \cdot \mathcal{C}_{\alpha}^{-1} \cdot \mathcal{D}_{\alpha}) \cdot (\mathcal{C}_{\alpha} + \mathrm{i}\omega \mathcal{D}_{\alpha})^{-1} \cdot \widehat{\mathcal{C}}.$

Stationarity system for the time-harmonic case

Global stationarity equations: A priori they read

$$
\int_{\Omega} (\boldsymbol{\sigma} : \boldsymbol{\varepsilon}[\overline{\hat{\boldsymbol{w}}}] - \rho \omega^2 \boldsymbol{u} \cdot \overline{\hat{\boldsymbol{w}}}) \, \mathrm{d}V = 0 \qquad \qquad \forall \, \hat{\boldsymbol{w}} \in \mathcal{W}.
$$

 \overline{a} $\frac{1}{\Omega}\left\{\left(\partial_\varepsilon\psi-\boldsymbol{\sigma}^\mathrm{e}-\mathrm{i}\omega T(\mathrm{i}\omega\partial_\varepsilon\varphi+\boldsymbol{\sigma}^\mathrm{v})\right):\varepsilon[\overline{\widehat{u}}]+\rho\omega^2\boldsymbol{w}\cdot\overline{\widehat{\boldsymbol{u}}}\right\}\,\mathrm{d}V=-\kappa\mathcal{D}(\boldsymbol{u}-\boldsymbol{u}_\mathrm{obs},\overline{\widehat{\boldsymbol{u}}})\qquad\forall~\widehat{\boldsymbol{u}}\in\mathcal{U}.$

• Use results from local stationarity, to obtain

$$
\int_{\Omega} \left\{ \left(\mathcal{C}(\omega) : \varepsilon[u] \right) : \varepsilon[\overline{\hat{w}}] - \rho \omega^2 u \cdot \overline{\hat{w}} \right\} dV + \int_{\Omega} \left(\mathcal{S}(\omega) : \varepsilon[w] \right) : \varepsilon[\overline{\hat{w}}] dV = 0 \qquad \forall \, \hat{w} \in \mathcal{W}
$$

$$
\int_{\Omega} \left(\left(\overline{\mathcal{C}(\omega)} : \varepsilon[w] \right) : \varepsilon[\overline{\hat{u}}] - \rho \omega^2 w \cdot \overline{\hat{u}} \right) dV - \kappa \mathcal{D}(u - u_{\text{obs}}, \overline{\hat{u}}) = 0 \qquad \forall \, \hat{u} \in \mathcal{U}
$$

• Stationarity system: perturbed mixed pb. (as in [Aquino, B 19] for time-harmonic elasticity)

 $S(\mathbf{w}, \widehat{\mathbf{w}}; \omega) + C(\mathbf{u}, \widehat{\mathbf{w}}; \omega) = 0 \qquad \forall \widehat{\mathbf{w}} \in \mathcal{W},$ $\overline{\mathsf{C}}(\boldsymbol{u},\widehat{\boldsymbol{u}};\omega) - \kappa \mathcal{D}(\boldsymbol{u},\widehat{\boldsymbol{u}}) = -\kappa \mathcal{D}(\boldsymbol{u}_{\mathrm{obs}},\overline{\widehat{\boldsymbol{u}}}) \qquad \forall \widehat{\boldsymbol{u}} \in \mathcal{U},$ $\mathsf{C}(\boldsymbol{u},\widehat{\boldsymbol{w}};\omega)=\big(\boldsymbol{\mathcal{C}}(\omega)\!:\!\boldsymbol{\varepsilon}[\boldsymbol{u}],\,\boldsymbol{\varepsilon}[\widehat{\boldsymbol{w}}]\big)_{\Omega}-\omega^2\big(\rho\boldsymbol{u},\,\widehat{\boldsymbol{w}}\big)_{\Omega},$ $\mathsf{S}(\boldsymbol{w},\widehat{\boldsymbol{u}};\omega)=\big(\boldsymbol{\mathcal{S}}(\omega)\!:\!\boldsymbol{\varepsilon}[\boldsymbol{w}],\,\boldsymbol{\varepsilon}[\widehat{\boldsymbol{w}}]\big)_{\Omega}$

• Key property: S coercive on $W \times W$.

[Transient or time-harmonic viscoelasticity](#page-39-0)

Numerical results (computations by P. Salasiya, B. Guzina)

- (possibly overlapping) subzones $\Omega = S_1 \cup \ldots \cup S_M$
- Identify heterogeneous p subzone-wise
- Computational experiments: 4 sources, 2 excitation directions each, 4 frequencies, $M = 4 \times 4$ square subzones
- Synthetic data generated with fine mesh $(h = .0025, p = 3);$
- Identification, stationarity solves etc. performed with coarser mesh ($h = .05$, $p = 3$), avoids "inverse crime";
- $\widetilde{\Lambda}_{\kappa}(\mathbf{p})$ minimized using SLSQP algorithm, p pixel-wise constant, $\mathcal{N} \times \mathcal{N}$ pizels per subzone, resolution refinement $\mathcal{N} = 1, 5, 7$.
- Noisy data: under progress, κ set by seeking the "corner" of ther L-curve.

following Tan et al. (2016), McGarry et al. (2022) for elastography

Numerical results (P. Salasiya, B. Guzina)

Isotropic standard linear solid model, $\mathbf{p} = (\kappa, \mu, \kappa', \mu', \eta, \chi)$

$$
\mathcal{C}(\mathbf{p},\omega)=\frac{3\kappa(\kappa'-\mathrm{i}\omega\eta)}{\kappa+\kappa'-\mathrm{i}\omega\eta}\mathcal{J}+\frac{2\mu(\mu'-\mathrm{i}\omega\chi)}{\mu+\mu'-\mathrm{i}\omega\chi}\mathcal{K},
$$

Numerical results (P. Salasiya, B. Guzina)

Kelvin-Voigt bulk approximation (due to $\eta \ll 1$):

 $1/8$

 \overline{D}

 $1/8$

 $\overline{1}$

- • Stationarity problem for the transient case:
	- \triangleright well-posedness results, conditions on the data?
	- ▷ potential computational bottleneck

Thank you for your kind attention! Any questions?