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Implicit port-Hamiltonian systems: structure-preserving discretization for the nonlocal vibrations in a viscoelastic nanorod, and for a seepage mode

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ANR IMPACTS :
Implicit port Hamiltonian control systems

Outline

Outline

Main objective

General purpose

Simulate complex multiphysics open systems while keeping some intrinsic physical properties such as the ***energy/power balance***

- *Finite Element Method:*
  → **Complex geometries** are allowed.
  → A wide range of **software** tools are available.

- *Port-Hamiltonian Systems (PHS):*
  → Keep track of **power exchanges** throughout the subsystems and with the environment
  → Intrinsic properties are encoded in a **Stokes-Dirac structure** and Hamiltonian function

- *Partitioned Finite Element Method (PFEM):*
  → It translates the Stokes-Dirac structure into a **Dirac structure**.
  → The **discrete Hamiltonian** satisfies the "discrete" power balance.

Main objective

Already many worked out examples (pHs and PFEM):

1. linear 2D wave PDE
2. Reissner-Mindlin or Kirchhoff-Love plate PDEs
3. 2D and 3D Maxwell's equations
4. 2D and 3D heat PDE, with internal energy or entropy as Hamiltonian
5. nonlinear 2D Shallow Water Equation, inviscid or viscous
6. nonlinear 2D Incompressible Navier-Stokes Equations
7. nonlinear 2D Allen-Cahn and Cahn-Hilliard PDEs

$\Longrightarrow$ Apply PFEM to a new class of models: *non-local* PDEs as *implicit* pHs:

1. a 1D example: nonlocal vibrations in a viscoelastic nanorod
2. a 2D example: the Dzektser seepage model

Outline

A 1D ex: nonlocal vibrations in a viscoelastic nanorod

In [Heidari & Zwart, 2019], the a wave PDE is considered, with a nonlocal constitutive equation between the stress σ and the strain ϵ

$$\sigma - \mu \frac{\partial^2 \sigma}{\partial x^2} = E(\epsilon + \tau_d \frac{\partial \epsilon}{\partial t}),$$

i.e. *the stress at a point is related to the strain at all other points in the domain* [Eringen, 1983].

The following Hamiltonian is considered

$$\mathcal{H} := \frac{1}{2} \int_\Omega \left(a^2 w^2 + \rho A \left(\frac{\partial w}{\partial t} \right)^2 + \mu \rho A \left(\frac{\partial^2 w}{\partial t \partial x} \right)^2 + (EA + \mu a^2) \left(\frac{\partial w}{\partial x} \right)^2 \right),$$

where $\mu > 0$ is the nonlocal parameter, and $\varepsilon := \sqrt{\mu}$ is the characteristic length of nonlocal effects.

Choosing $z := \begin{pmatrix} w, & \rho A \frac{\partial w}{\partial t}, & \mu \rho A \frac{\partial^2 w}{\partial t \partial x}, & \frac{\partial w}{\partial x}, & N \end{pmatrix}^\top$ as energy variables, and denoting

$$\mathbb{E} := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad Q := \begin{pmatrix} a^2 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\rho A} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\mu \rho A} & 0 & 0 \\ 0 & 0 & 0 & EA + \mu a^2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

the Hamiltonian $\mathcal{H}$ rewrites $\mathcal{H} = \frac{1}{2} \int_\Omega z^\top \mathbb{E}^\top Q z$, with the important algebraic property $\mathbb{E}^\top Q = Q^\top \mathbb{E}$.

The dynamics of the system is given by

$$\mathbb{E} \dot{z}(t) = (J - R) e(t), \qquad e = Qz \tag{1}$$

$$J := \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & \frac{\partial}{\partial x} \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & \frac{\partial}{\partial x} & -1 & 0 & 0 \end{pmatrix}, \quad R := \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & b^2 & 0 & 0 & 0 \\ 0 & 0 & \tau_d EA + \mu b^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The power balance reads:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(t) = -\int_{\Omega} e(t,x)\cdot Re(t,x)\mathrm{d}x + [u(t,s)y(t,s)]_0^{\ell}, \leq [u(t,s)y(t,s)]_0^{\ell}, \tag{2}$$

where u and y stand for boundary control and boundary observation. More precisely, let us recall $e_2 = \frac{\partial w}{\partial t}$ and $e_5 = N$. Therefore the boundary product of the control and the observation must result in the product between the **velocity** and the **force** at the boundary: $u = N, y = \frac{\partial w}{\partial t}$.

$\Rightarrow$ The descriptor dynamical system is lossy.

Outline

The PFEM strategy

1. Write the **weak formulation**;
2. Apply an appropriate **Stokes identity** (such that the chosen boundary control u "appears");
3. Project on a finite-dimensional space thanks to **FEM**.

Discretization of the structure and of the constitutive relations are made separately.

The discretized system is:

$$\begin{cases} \mathbf{M}_q \cdot \frac{\mathrm{d}}{\mathrm{d}t}\underline{\alpha}_q(t) = D \cdot \underline{e}_p(t) + B \cdot \underline{u}(t), \\ M_p \cdot \frac{\mathrm{d}}{\mathrm{d}t}\underline{\alpha}_p(t) = -D^\top \cdot \underline{e}_q(t), \\ M_\partial \cdot \underline{y}(t) = B^\top \cdot \underline{e}_q(t), \end{cases}$$

together with (linear case)

$$\begin{cases} \mathbf{M}_q \cdot \underline{e}_q(t) = \mathbf{M}_{\underline{\underline{\boldsymbol{T}}}} \cdot \underline{\alpha}_q(t), \\ M_p \cdot \underline{e}_p(t) = M_{\frac{1}{\rho}} \cdot \underline{\alpha}_p(t) \end{cases}$$

$\Longrightarrow$ in general, PFEM for pHs gives rise to finite-dimensional PH-DAEs involving (quite often) **sparse matrices** only, and for which **efficient numerical methods** can be used.

On the nanorod model as a pHs, we get:

$$\left\{\begin{array}{rcl} \mathbf{E}\dot{\underline{z}}(t) & = & (\mathbf{J}-\mathbf{R})\,\underline{e}(t)+\mathbf{B}\underline{u}(t), \\ \mathbf{M}\underline{e}(t) & = & \mathbf{Q}\underline{z}(t), \\ \underline{y}(t) & = & \mathbf{B}^\top\underline{e}(t). \end{array}\right. \tag{3}$$

The algebraic property $\mathbb{E}^\top Q = Q^\top\mathbb{E}$ translates into $\mathbf{E}^\top\mathbf{M}^{-1}\mathbf{Q} = \mathbf{Q}\mathbf{M}^{-1}\mathbf{E}$.

The discrete power balance reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}^d(t) = -\underline{e}(t)^\top\mathbf{R}\underline{e}(t) + \underline{u}(t)^\top\underline{y}(t) \leq \underline{u}(t)^\top\underline{y}(t),$$

and is the discrete counterpart of (2).

Outline

simulation results with SCRIMP

Difference between the local model ($\mu = 0.001$), and the nonlocal model ($\mu = 0.01$)

$\Longrightarrow$ More about SCRIMP environment: `https://g-haine.github.io/scrimp/`

simulation results with SCRIMP

Role of non-local parameter μ: $\mu = 0.1$, $\mu = 0.5$ and $\mu = 2$.

Outline

A 2D example: the Dzektser seepage model

From Dzektser, E.S. (1972): *Generalization of the equation of motion of ground waters with free surface*. Dokl. Akad. Nauk SSSR, 202(5), 1031–1033.

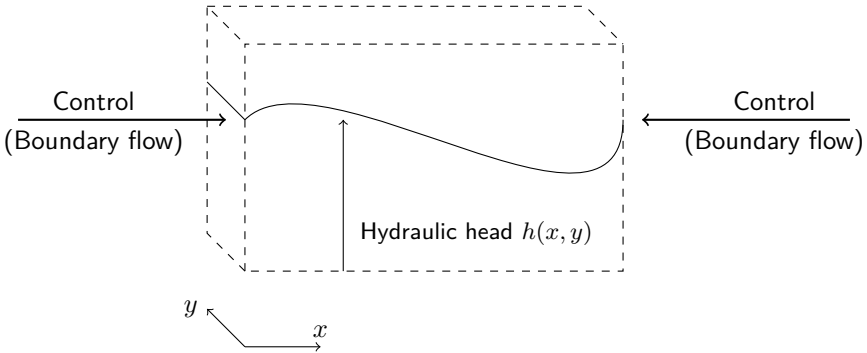


Figure: Underground water seepage model

A 2D example: the Dzektser seepage model

Let us define $\bar{h_0} > 0$ the mean hydraulic head, μ the coefficient of free porosity, k the permeability of the medium, ϵ_0 and ϵ_a the quantities for feeding the flow through its base and free surface.

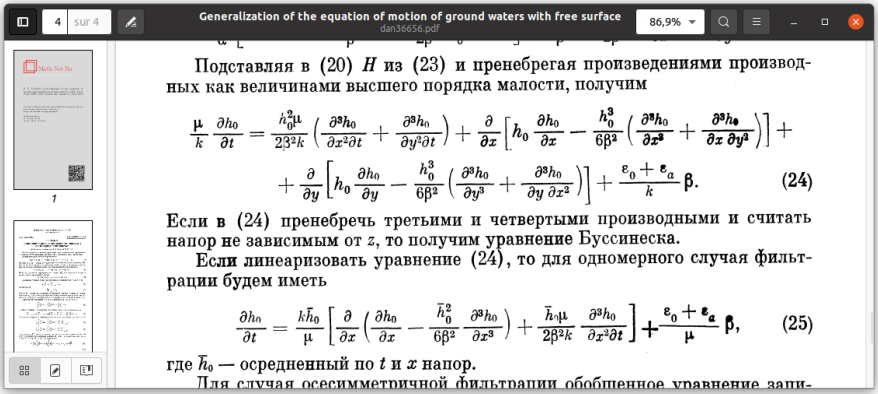
The evolution of the hydraulic head h_0 is governed by the following implicit PDE:

$$(1 - \varepsilon^2 \Delta) \frac{\partial h_0}{\partial t} = a\, \Delta h_0 - b\, \Delta^2 h_0 + \frac{\epsilon_0 + \epsilon_a}{\mu}\, \beta,$$

where $\varepsilon := \frac{\bar{h}_0}{\sqrt{2}\beta}$ is the *characteristic length* of the nonlocal effect, $a = \frac{k}{\mu}\bar{h_0}$, and $b = \frac{\bar{h_0}^2}{6\beta^2} a$ are the adimensional damping parameters

In the sequel we will consider $\epsilon_0 = \epsilon_a = 0$, and a control at the boundary of the 2D horizontal domain.

A 2D example: the Dzektser seepage model



Note that the minus sign in front of the Laplacian operator is to be found in eq (24) of [Dzektser, 1972], and cited as such in e.g. [Perevozhikova and Manakova, (2021)].
However, in several related works, it has been transformed into a plus sign, giving rise to a singularity, since in this case the unbounded differential operator has a nonzero kernel, a mathematical artifact which is not based on any physical ground.

Let us introduce a classical Hamiltonian in *nonlocal mechanics*:

$$\mathcal{H} = \frac{1}{2}\int_\Omega {h_0}^2 + \varepsilon^2 \left\|\mathbf{grad}(h_0)\right\|^2. \tag{4}$$

see e.g. *ASTER Code*, a simulation environment for EDF (Electricité De France).

The power balance reads:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H} = -\int_\Omega a \left\|\mathbf{grad}(h_0)\right\|^2 - \int_\Omega b\,(\Delta h_0)^2 + \int_{\partial\Omega} \boldsymbol{u}_\partial^\top\, \boldsymbol{y}_\partial \leq \int_{\partial\Omega} \boldsymbol{u}_\partial^\top\, \boldsymbol{y}_\partial \tag{5}$$

with appropriate collocated boundary controls and observations.

The boundary controls $\boldsymbol{u}_\partial$ consist of the flux $u_f := (a\,\mathbf{grad}(h_0) - b\,\mathbf{grad}(\Delta h_0))\cdot\boldsymbol{n}$, the pressure $u_p := \mathbf{grad}(h_0)\cdot\boldsymbol{n}$ and the pressure *derivative* $\partial_t u_p = \mathbf{grad}\left(\frac{\partial h_0}{\partial t}\right)\cdot\boldsymbol{n}$.

The **lossy** dynamical system can be reformulated in the following way, making use of **extra dissipation ports**:

$$\begin{pmatrix} (1-\varepsilon^2\Delta)\frac{\partial h_0}{\partial t} \\ \mathbf{grad}(h_0) \\ \Delta h_0 \end{pmatrix} = \begin{pmatrix} 0 & \mathrm{div} & -\Delta \\ \mathbf{grad} & 0 & 0 \\ \Delta & 0 & 0 \end{pmatrix} \begin{pmatrix} h_0 \\ a\,\mathbf{grad}(h_0) \\ b\,\Delta h_0 \end{pmatrix}. \tag{6}$$

In (6), the Laplacian operator in front of the time derivative $\partial_t h_0$ is very reminiscent of a similar situation for the numerical treatment of the Incompressible Navier-Stokes equations, studied e.g. in [Haine and Matignon, 2021]. Indeed in this latter case, minus the Laplacian operator was included in the constitutive equations relating the vorticity ω and the stream function ψ.

The appearance of the time derivative of the boundary control is related to the index 2 of the underlying Differential Algebraic Equation (DAE), see e.g. [Mehrmann and Unger, 2023] and references therein.

Outline

With a mass matrix given by $\mathbf{M}_\varepsilon := \mathrm{diag}(\mathbf{M}_1 + \varepsilon^2\mathbf{K}, \mathbf{M}_{\boldsymbol{\phi}}, \mathbf{M}_2)$, the finite-dimensional pHs reads:

$$\begin{cases} \mathbf{M}_\varepsilon \begin{pmatrix} \frac{d}{dt}\underline{h}_0 \\ \underline{f}_{\mathbf{grad}} \\ \underline{f}_\Delta \end{pmatrix} = \mathbf{J} \begin{pmatrix} \underline{h}_0 \\ \underline{e}_{\mathbf{grad}} \\ \underline{e}_\Delta \end{pmatrix} + \begin{pmatrix} \mathbf{B}_f & 0 & \varepsilon^2\mathbf{B}_{p,1} \\ 0 & 0 & 0 \\ 0 & \mathbf{B}_{p,2} & 0 \end{pmatrix} \begin{pmatrix} \underline{u}_f \\ \underline{u}_p \\ \frac{d}{dt}\underline{u}_p \end{pmatrix}, \\ \begin{pmatrix} \mathbf{M}_{\boldsymbol{\phi}} & 0 \\ 0 & \mathbf{M}_2 \end{pmatrix} \begin{pmatrix} \underline{e}_{\mathbf{grad}} \\ \underline{e}_\Delta \end{pmatrix} = \begin{pmatrix} \mathbf{C}_a & 0 \\ 0 & \mathbf{C}_b \end{pmatrix} \begin{pmatrix} \underline{f}_{\mathbf{grad}} \\ \underline{f}_\Delta \end{pmatrix}, \end{cases}$$

$$\begin{pmatrix} \mathbf{M}_f^\partial & 0 & 0 \\ 0 & \mathbf{M}_p^\partial & 0 \\ 0 & 0 & \mathbf{M}_p^\partial \end{pmatrix} \begin{pmatrix} \underline{y}_f \\ \underline{y}_p \\ \underline{y}_{\mathrm{d}_t p} \end{pmatrix} = \begin{pmatrix} \mathbf{B}_f^\top & 0 & 0 \\ 0 & 0 & \mathbf{B}_{p,2}^\top \\ \varepsilon^2\mathbf{B}_{p,1}^\top & 0 & 0 \end{pmatrix} \begin{pmatrix} \underline{h}_0 \\ \underline{e}_{\mathbf{grad}} \\ \underline{e}_\Delta \end{pmatrix}.$$

The discrete Hamiltonian is defined by:

$$\mathcal{H}^{\mathrm{d}} := \frac{1}{2}\int_{\Omega} (h_0^d)^2 \; + \varepsilon^2 \|\mathbf{grad} h_0^d\|^2 = \frac{1}{2}(\underline{h_0}^{\top}\mathbf{M}_1\underline{h_0} + \varepsilon^2 \underline{h_0}^{\top}\mathbf{K}\underline{h_0}).$$

The discrete power balance reads:

$$\begin{aligned}
\frac{d}{dt}\mathcal{H}^{\mathrm{d}} &= \frac{d}{dt}(\frac{1}{2}(\underline{h_0}^{\top}\mathbf{M}_1\underline{h_0} + \underline{h_0}^{\top}\varepsilon^2\mathbf{K}\underline{h_0}) && (7)\\
&= -a\,\underline{f}_{\mathbf{grad}}^{\top}\,\mathbf{M}_{\boldsymbol{\phi}}\,\underline{f}_{\mathbf{grad}} - b\,\underline{f}_{\Delta}^{\top}\,\mathbf{M}_2\,\underline{f}_{\Delta} + \underline{e}_{\Delta}^{\top}\,\mathbf{B}_{p,2}\,\underline{u}_p + \underline{h}_0^{\top}\,\mathbf{B}_f\,\underline{u}_f + \varepsilon^2\underline{h}_0^{\top}\,\mathbf{B}_{p,1}\,\frac{d}{dt}\underline{u}_p, && (8)\\
&\leq \underline{y}_{\partial}^{\top}\,\mathbf{M}^{\partial}\,\underline{u}_{\partial} && (9)
\end{aligned}$$

$\Longrightarrow$ the finite-dimensional pHs is also lossy.

Outline

simulation results with SCRIMP

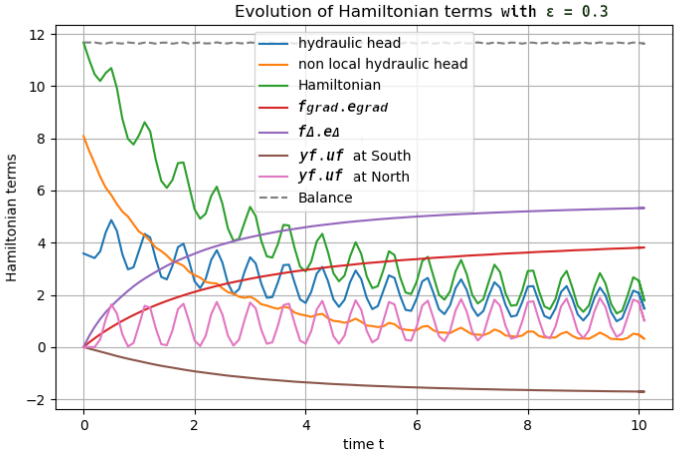


Figure: $T = 10$, $dt = 0.1$, $a = 0.01$, $b = 0.0001$, $\varepsilon = 0.3$

simulation results with SCRIMP

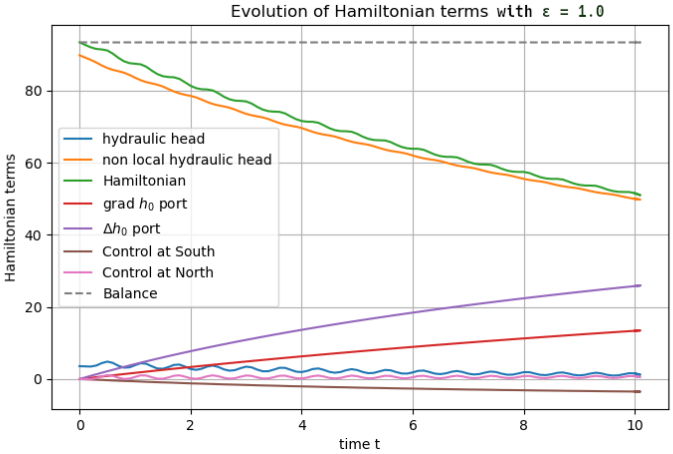


Figure: $T = 10$, $dt = 0.1$, $a = 0.01$, $b = 0.0001$, $\varepsilon = 1.0$

simulation results with SCRIMP

$\Longrightarrow$ More about SCRIMP environment: `https://g-haine.github.io/scrimp/`

Outline

Conclusion, Outlook & Bibliography

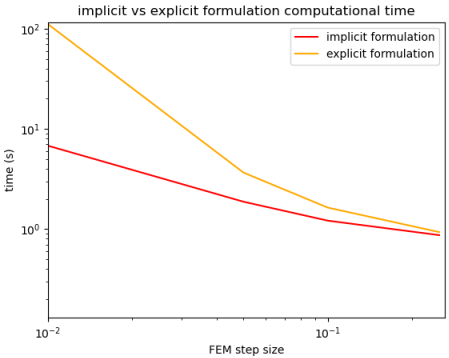
PFEM provides a systematic way to discretize a large class of **port-Hamiltonian systems in a structure-preserving manner**.

Furthermore, dissipative systems can easily be tackled by PFEM (with additional DAEs).

The method enjoys:

- a mimetic power balance and modularity;
- a well-known and robust theory of FE;
- low requirement on the choices of FE families;
- specialized numerical linear algebra for sparse matrices;
- the wide range of FE libraries.

Outlook: pros and cons of the two formulations (1/2)



In [Heidari & Zwart, 2019], a *second* Hamiltonian functional is proposed, involving G a symmetric integral operator: it gives rise to a pH-ODE. The compact operator G is making explicit the implicit part $(1 - \mu \frac{d^2}{dx^2})$ of the original pH-DAE formulation.

$\Rightarrow$ Applying PFEM leads to a $\mathbf{G}$ matrix which is dense, and no more sparse, as the discrete counterpart of the G operator: thus, one has to deal with an increased computational burden.

Outlook: pros and cons of the two formulations (2/2)

The difference between the explicit formulation, and the implicit formulation comes from the associated boundary conditions.

$\Longrightarrow$ Taking them into account should prove possible, thanks to the *Stokes-Lagrange* framework, following e.g. [van der Schaft & Maschke, 2018] or [Maschke & van der Schaft, 2023].

Outlook: a parameterized family of nonlocal models

The appearance of the particular $I - \varepsilon^2 \Delta$ operator in both the implicit models delt with so far is strongly linked to the choice of the nonlocal kernel, of the form $\exp(-\|x\|/\varepsilon)$, see [Eringen, 1983].

$\Longrightarrow$ What kind of implicit models would appear with the choice of other nonlocal kernels? Could a hierarchy of such models or families be built?

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