Partially mesoscopic and Lagrangian systems

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AG Differential-Algebraische Systeme
FB Mathematik
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The principle question

$$\begin{cases} L & := \underbrace{L_0(r,\dot r)}_{\text{heavy}} + \sum_{j=1}^{n} \underbrace{L_1(q_j,\dot q_j)}_{\text{particles}} \\ g(r,q_j) & = \text{const.} \end{cases}$$

for large values of n, we need statistical ensembles...

	Euler-Lagrange equation	Partially mesoscopic system	Liouville equation
unknowns	$r, \dot r, q_j, \lambda_j$	$r, \dot r, \rho(q,t), \lambda(q)$	$\rho(r, \dot r, q, t)$

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1. Derivation of partially mesoscopic system
2. Numerical experiments (conservative case)
3. Original motivation: mechanics of muscle tissue
4. Numerical challenges (non-conservative case)

Point of Departure

The equation of motion are given by

$$M_0 \ddot{r} = -\partial_r L_0(r, \dot{r}) - \sum_{i=1}^{n} \lambda_i \partial_r g(r, q_i), \quad (1)$$

$$M_1 \ddot{q}_j = -\partial_q L_1(q_j, \dot{q}_j) - \lambda_j \partial_q g(r, q_j), \quad (2)$$

$$0 = g(r, q_j) - c_j, \quad \text{for all } j = 1, \dots n. \quad (3)$$

The same constraint function $g(r, q)$ for all n particles! But c_j depends on the initial conditions.

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Main assumption

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$\rightarrow$ the state of the heavy system $(r,\dot{r})$ determines at least locally the complete state $(r,\dot{r},\dots,q_j(r),\dot{q}_j(r,\dot{r}),\dots)$!

Toy example

We consider a very heavy spring

$$L_0(r, \dot{r}) = \frac{1}{2} m_0 \dot{r}^2 + \frac{1}{2} \kappa_0 r^2$$

and many very light springs

$$\frac{1}{n} L_1(q, \dot{q}) = \frac{1}{2} \frac{m_1}{n} \dot{q}^2 + \frac{1}{2} \frac{\kappa_1}{n} q^2$$

combined as

$$L = L_0 + \frac{1}{n} \sum_{j=1}^{n} L_1, \quad g(r, q_j) = r - q_j - \underbrace{(r(0) - q_j(0))}_{=:c_j}.$$

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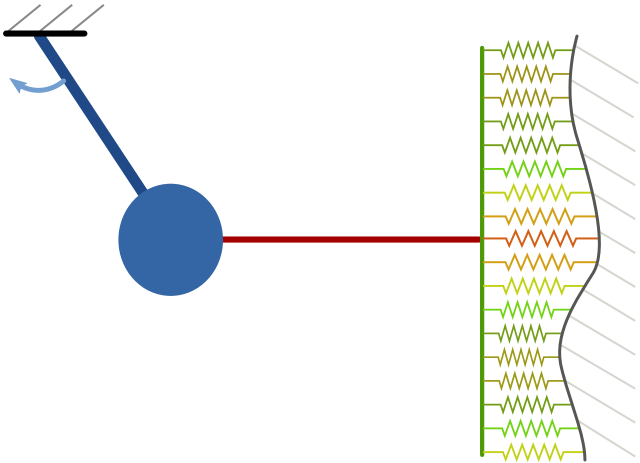

heavy system constraint particles

Recall: Liouville's equation

If we consider a (arbitrary) Hamilton system $H(q,p)$ and an initial density $\rho_0(q,p)$, then the evolution of

$$\rho(q(t),p(t),t) := \rho_0(q(0),p(0))$$

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Liouville equation of the complete system.

The Liouville equation for

$$L := L_0 + L_1, \qquad g = 0$$

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$$0 = \partial_r g \dot{r} + \partial_q g \dot{q}. \tag{7}$$

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Equation of partially mesoscopic systems

$$M_0 \ddot{r} = -\partial_r L_0 - \int \lambda(q) \partial_r g(r, q) \rho(q, t) \, \mathrm{d}q, \quad (8)$$

$$\partial_t \rho + v_1(\dot{r}) \, \partial_q \rho = 0, \quad (9)$$

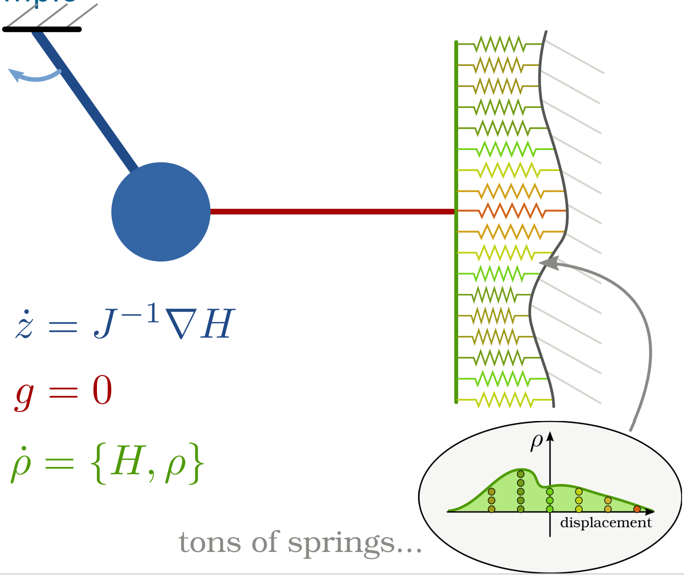
$$\lambda(q) \partial_q g = M_1 a_1(\ddot{r}) + \partial_q L_1 \quad (10)$$

with the definition

$$v_1(\dot{r}; q, r) := -\left(\partial_q g\right)^{-1} \partial_r g[\dot{r}], \quad (11)$$

$$a_1(\ddot{r}; q, r, \dot{r}) := -(\partial_q g)^{-1} \Big(\partial_r^2 g[\dot{r}, \dot{r}] + 2 \partial_r \partial_q g\big[\dot{r}, v_1(\dot{r})\big] \partial_q^2 g\big[v_1(\dot{r}), v_1(\dot{r})\big] + \partial_r g[\ddot{r}] \Big). \quad (12)$$

Toy example



$$\dot{z} = J^{-1}\nabla H$$

$$g = 0$$

$$\dot{\rho} = \{H, \rho\}$$

tons of springs...

Clash of numerical philosophies...

- We have classical physical system

$$M_0 \ddot{r} = -\partial_r L_0 - \int \lambda(q) \partial_r g(r,q) \rho(q,t) \, \mathrm{d}q.$$

$\Rightarrow$ maybe symplectic methods?

- There is a conservation law

$$\partial_t \rho + v_1(\dot{r}) \, \partial_q \rho = 0.$$

$\Rightarrow$ maybe upwind? Or more complicated?

- And it is still a DAE of Index 1

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- **Semi-Lagrangian approach:** If g is linear w.r.t. q, then we just need to approximate the shift

$$h(t) = \int_0 v_1(s)\,\mathrm{d}s.$$

and set

$$\rho(q,t) = \rho(q - h(t), 0).$$

  - $h(t)$ can be integrated in a symplectic manner!
- **Upwind:** Boundary conditions for the conservation law are missing!
  - It is unclear how symplectic methods are defined for the integration of the conservation law.

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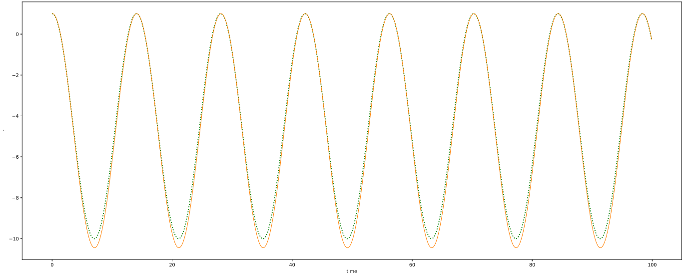
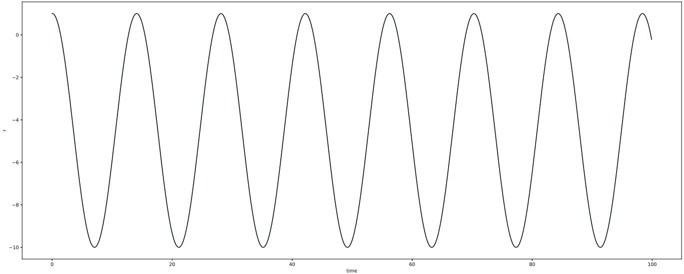
Toy-Example: Euler-Lagrange vs. Partially Mesoscopic

If the initial values q_j are normally distributed, a direct simulation or a Monte-Carlo simulation requires far more degrees of freedom ($n \approx 10^4$) for good convergence, compared to a semi-Lagrangian scheme ($n_\rho \approx 30$).

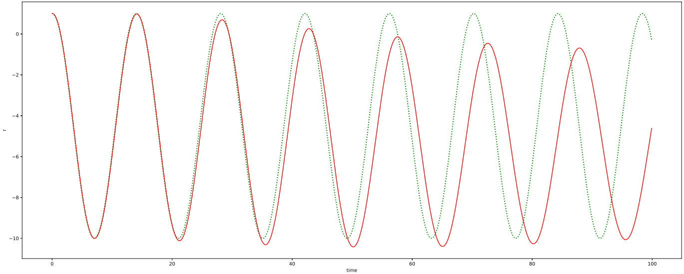
Euler-Lagrange, Monte-Carlo



Semi-Lagrangian Approach



Upwind



Muscle tissue

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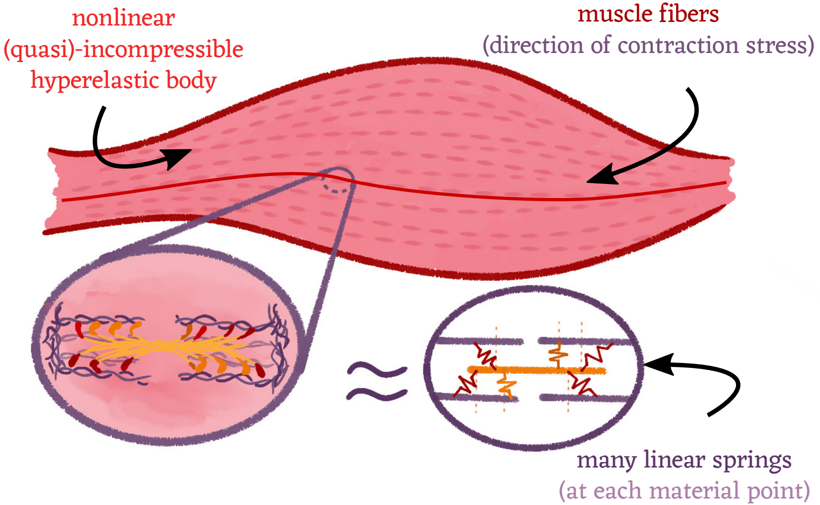

Basically same, but a tiny little bit infinite dimensional

- **Heavy system** '$L_0(u, \nabla u, \dot{u}; X, t)$': Nonlinear quasi-incompressible hyperelastic solid. (Classical field theory)
- **Particle systems** '$\sum_j L_1(q_j(X), \dot{q}_j(X), t)$': Actin-Myosin cross-bridges in each sarcomere (muscle cell).
- **Constraints** '$g(u(X), \nabla u(X), q_j(X)) = 0$' for all material points X and all particles j.

Classical field theory fits nicely to this theory

Muscles as a "partially mesoscopic system"

$$m_0\ddot{\varphi} = \operatorname{Div}(\boldsymbol{P} - \lambda \boldsymbol{G}),$$

$$\partial_t \rho - v_1 \partial_q \rho_q = 0,$$

$$\lambda \boldsymbol{G} := \int_{\mathbb{R}} \lambda(q) \boldsymbol{G} \rho(q)\, \mathrm{d}q,$$

$$\lambda(q) := \kappa_1 q - m_1 \frac{\mathrm{d}^2}{\mathrm{d}t^2} \|n_{\mathrm{fiber}}\|,$$

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The Lagrangian multiplier is a scalar field, defining strength of the active contraction stress.

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Non-conservative part of muscle models!

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Numerical challenges

- Source terms in the transport equation

$$\partial_t \rho - v_1 \partial_q \rho = f \cdot (1 - \rho) + g \cdot \rho,$$

lead to a stiff system!

  - Semi-Lagrangian integration is unstable for discontinuous $f(q), g(q)$.

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  - Modeling as a Port-Hamiltonian system possible?!

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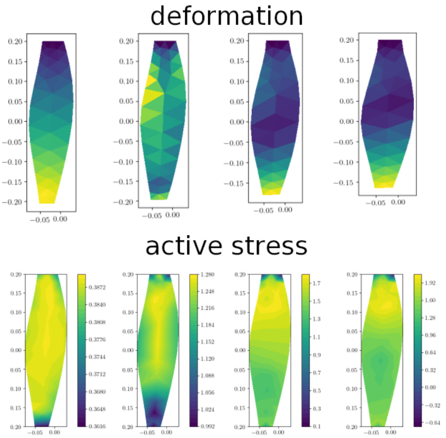
Colourful but unstable for large deformations...



Conclusion

- We developed a framework for coupling between classical Lagrangian and mesoscopic systems.
- Naive, simple and computational efficient methods for the conservative case are available.
- The non-conservative case is numerically difficult: **a mix between different numerical philosophies is required.**
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Thanks for your attention!