Dynamic Instabilities caused by Reaction Cross-Diffusion Waves in Porous Media

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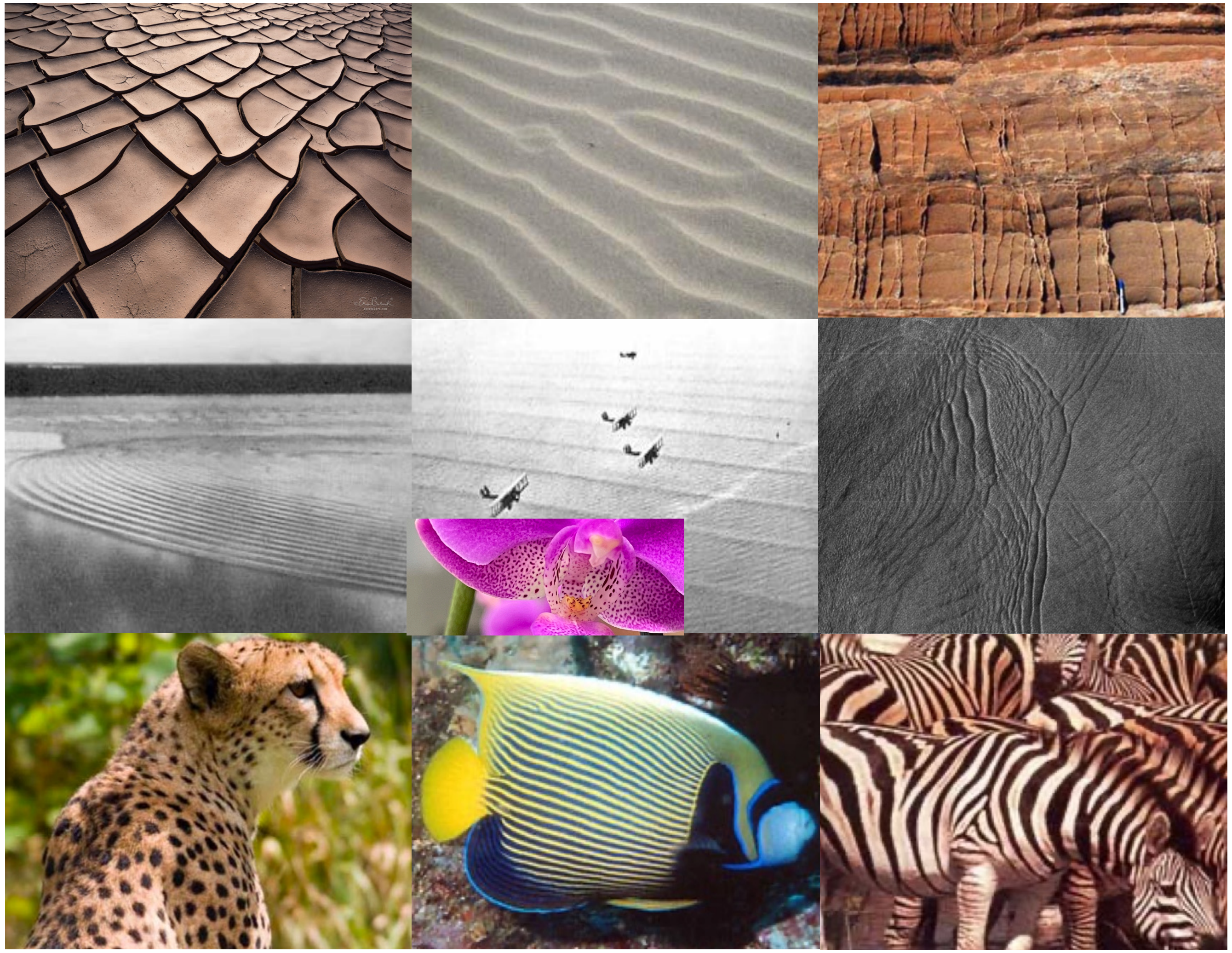
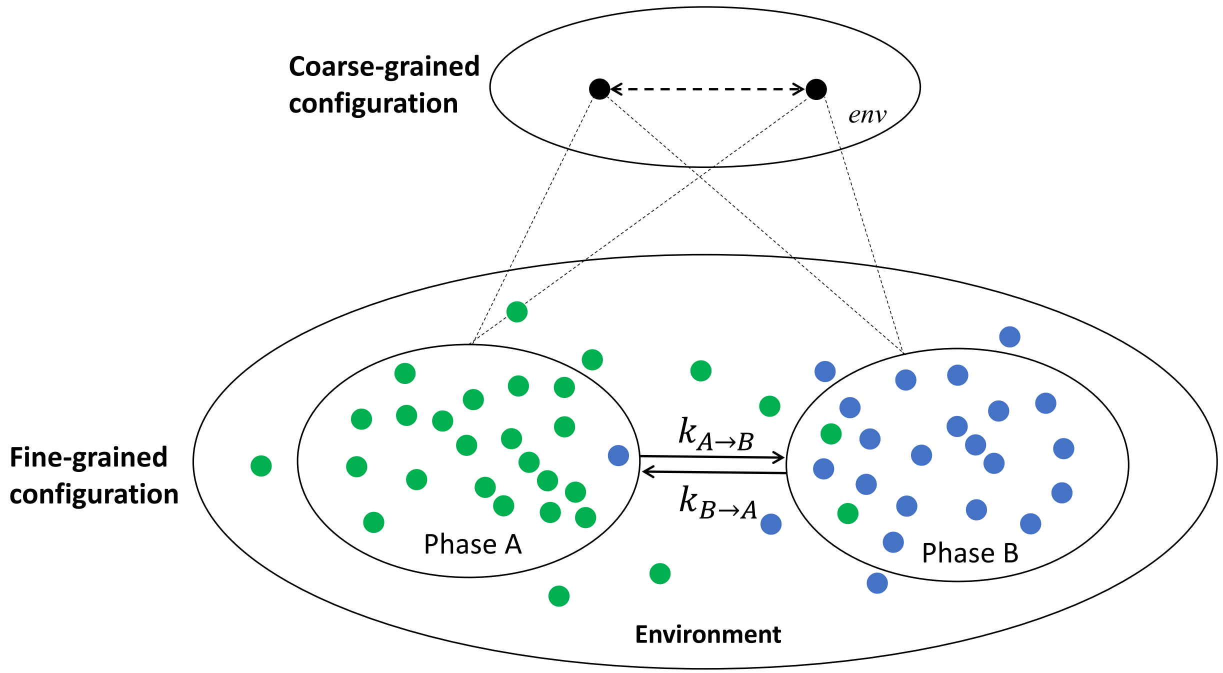
Patterns in nature



- Thermodynamics allows prediction of the final state with the dynamic evolution of the micro-processes refrained.

Cross-diffusion in a poromechanical system

- **Cross-diffusion** in general (e.g., in chemistry) describes the interaction of at least two entities where the thermodynamic *flux* (mass flow of species) is cross-coupled to the thermodynamic *force* (concentration gradient) of another kind.
- Considering this type of *cause and effect*, the master reaction-diffusion equation has additional cross-diffusion terms.
- We borrow this concept to describe a generic system behaviour of hydromechanically coupled porous media (abstracted as a **dual-continuum**).



- In the sense of hydromechanics:

Thermodynamic force	Thermodynamic flux
pressure difference in the fluid/solid phase	mass flux from the fluid/solid phase

$$\frac{dC_{\mathrm{A}}}{dt} = \nabla(\bar{D}_{\mathrm{AA}}\nabla C_{\mathrm{A}}) + \nabla(\bar{D}_{\mathrm{AB}}\nabla C_{\mathrm{B}}) + r_{\mathrm{A}}$$

$$\frac{dC_{\mathrm{B}}}{dt} = \nabla(\bar{D}_{\mathrm{BA}}\nabla C_{\mathrm{A}}) + \nabla(\bar{D}_{\mathrm{BB}}\nabla C_{\mathrm{B}}) + r_{\mathrm{B}}$$

Introducing new non-local terms to the coarse-grained model

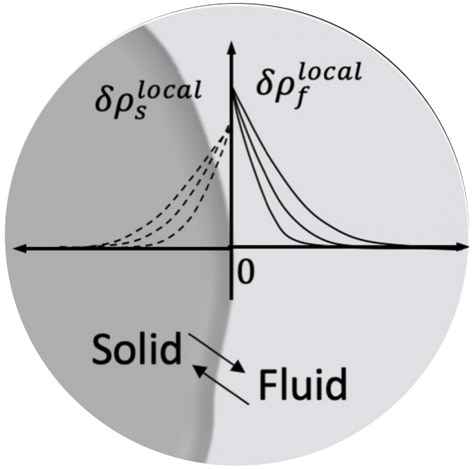
$$\frac{\partial \tilde{p}_s}{\partial \tilde{t}} = \underbrace{\nabla\cdot(\tilde{D}_M \nabla \tilde{p}_s)}_{Self-diffusion} + \underbrace{\nabla\cdot(\tilde{d}_H \nabla \tilde{p}_f)}_{Cross-diffusion} + \tilde{R}_1$$

(solid skeleton)

Non-local signature: cross-diffusion from volume integral over domain

$$\frac{\partial \tilde{p}_f}{\partial \tilde{t}} = \underbrace{\nabla\cdot(\tilde{d}_M \nabla \tilde{p}_s)}_{Cross-diffusion} + \underbrace{\nabla\cdot(\tilde{D}_H \nabla \tilde{p}_f)}_{Self-diffusion} + \tilde{R}_2$$

(fluid)



Mixture theory + Inter-constituent mass transfer + Relaxing the adiabatic constraints

- The fluid reaction term $\tilde{R}_2$ is assumed to be linear (minerals' dehydration/rehydration) :

$$\tilde{R}_2 = \tilde{a}_{21}\tilde{p}_s + \tilde{a}_{22}\tilde{p}_f$$

- But the solid $\tilde{R}_1$ contains higher order terms of $\tilde{P}_s$ viscoplastic behavior of skeleton

$$\tilde{R}_1 = \tilde{a}_{11}\tilde{p}_s + \tilde{a}_{12}\tilde{p}_s^2 + \tilde{a}_{13}\tilde{p}_s^3 + \tilde{a}_{14}\tilde{p}_f$$

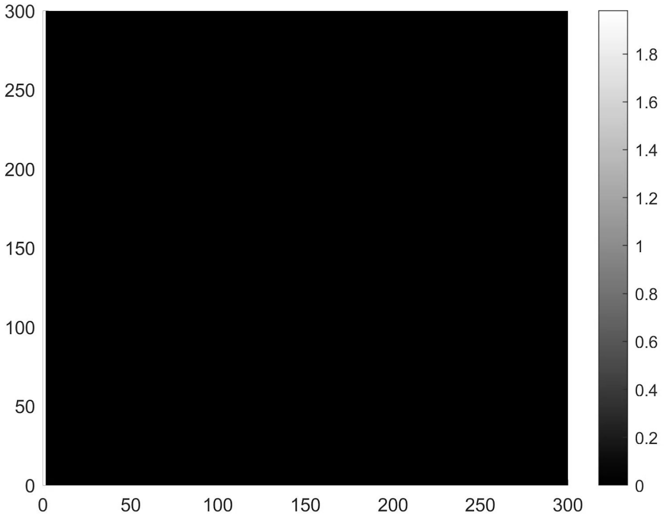
Non-local reaction (higher order approach)

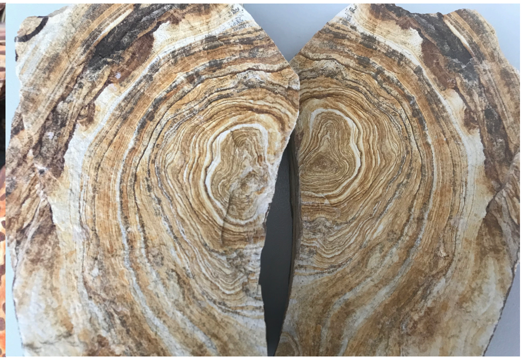
Originally proposed by Hu, Schrank and Regenauer-Lieb (JMPS 2020) https://doi.org/10.1016/j.jmps.2019.05.015

Varying parameters…. a rich world of waves

1. Singular spikes or spatially periodic (time independent) TURING PATTERNS

$$\frac{\widetilde{D}_M}{\widetilde{D}_H} > 12.7$$

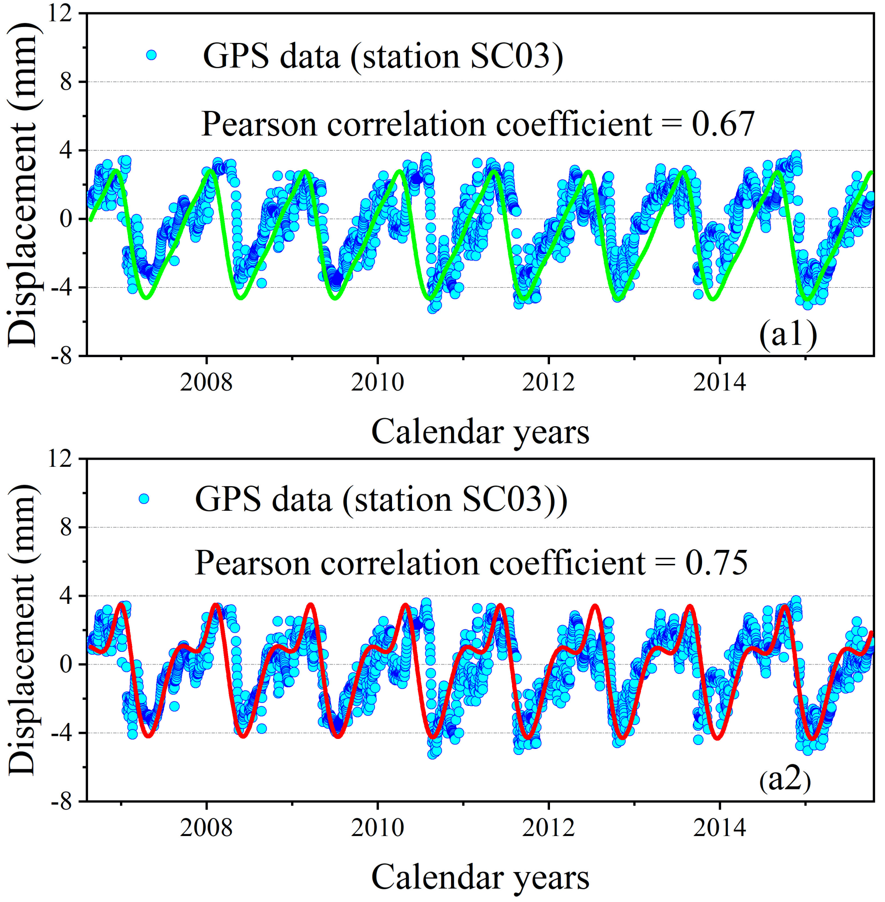




Varying parameters…. a rich world of waves

2. Time periodic Hopf Instabilities with

$$\tilde{f}_{k=0,1,2\cdots} = \frac{1}{\tilde{T}_k} \approx \frac{k\sqrt{4(\tilde{a}_{11}\tilde{a}_{22} - \tilde{a}_{14}\tilde{a}_{21}) - (\tilde{a}_{11} + \tilde{a}_{22})^2}}{4\pi}$$



Episodic Tremor and Slip Sequences modelled by the poromechanical reaction-cross-diffusion equation for serpentinite dehydration.

Hu, M., Q. Sun, C. Schrank and K. Regenauer-Lieb (2022). "Cross-scale dynamic interactions in compacting porous media as a trigger to pattern formation." Geophysical Journal International **230**(2): 1280-1291.

Discovery of a new dissipative wave in an excitable system

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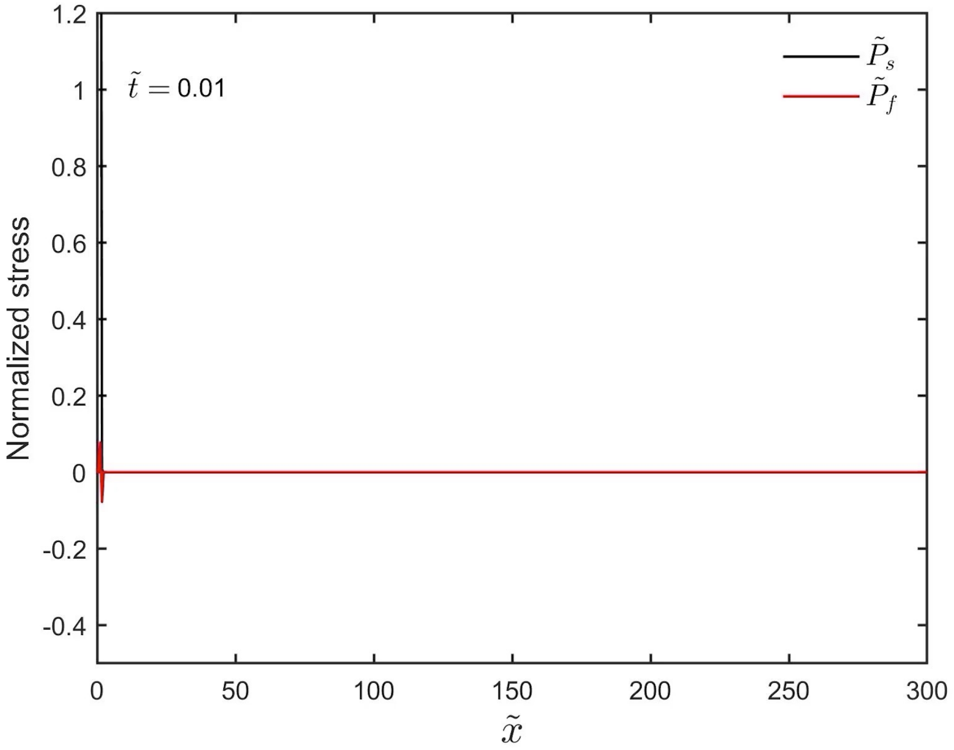
3. New Cross-diffusion waves

- The approach predicts solitary waves such as porosity waves.
- The addition of the explicit interaction between solids and fluids generates a new type of strongly dispersive soliton-like waves that *unlike solitons* are:
  - Independent of initial conditions.
  - Only depend on material properties.
  - Can pick up information such as system size from collision with boundaries.
  - Upon collision they can interact with themselves (not elastic).
  - They can couple multiphysics processes across scale.
  - Thereby providing the means to couple instabilities from the small to the large scale.

In 1-D:

$$\frac{\partial \tilde{p}_s}{\partial \tilde{t}} = \tilde{D}_M \frac{\partial^2 \tilde{p}_s}{\partial \tilde{x}^2} + \tilde{d}_H \frac{\partial^2 \tilde{p}_f}{\partial \tilde{x}^2} + \tilde{R}_1$$

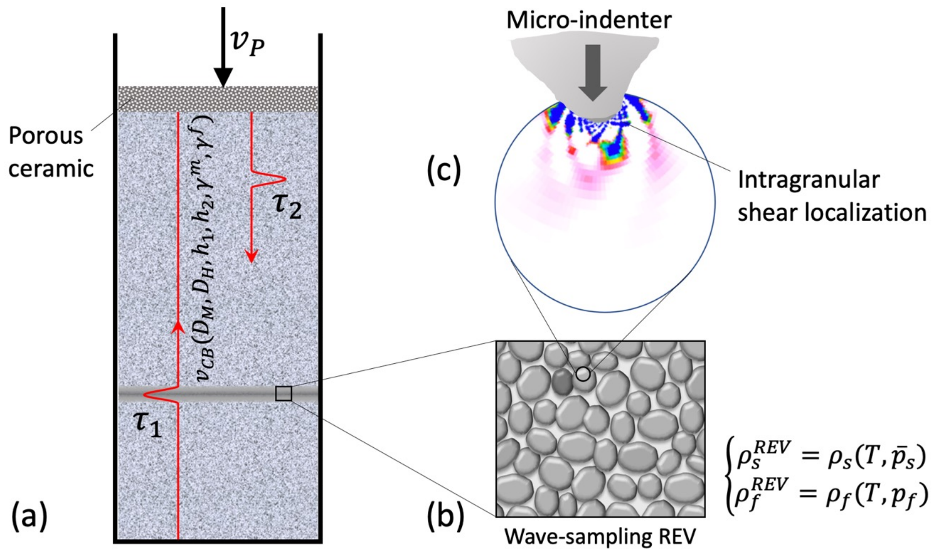
$$\frac{\partial \tilde{p}_f}{\partial \tilde{t}} = \tilde{d}_M \frac{\partial^2 \tilde{p}_s}{\partial \tilde{x}^2} + \tilde{D}_H \frac{\partial^2 \tilde{p}_f}{\partial \tilde{x}^2} + \tilde{R}_2$$

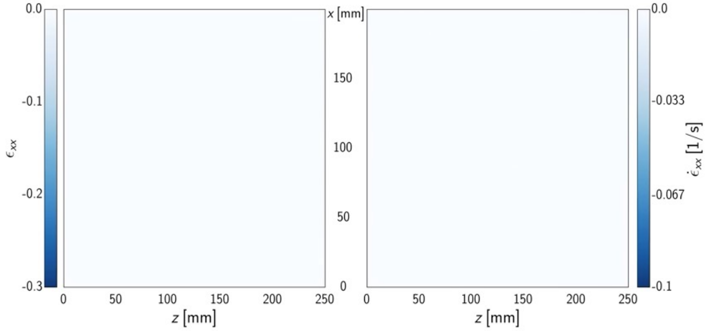


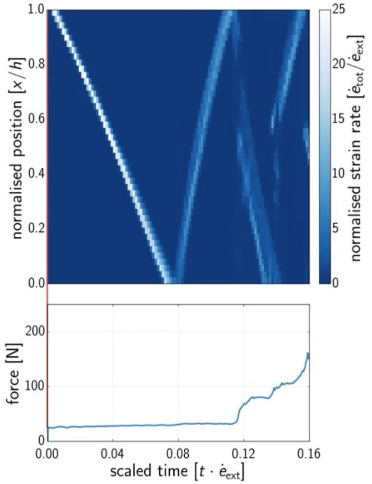
Regenauer-Lieb, Hu, et al., (SE 2021a, b)
https://doi.org/10.5194/se-12-869-2021
https://doi.org/10.5194/se-12-1829-2021

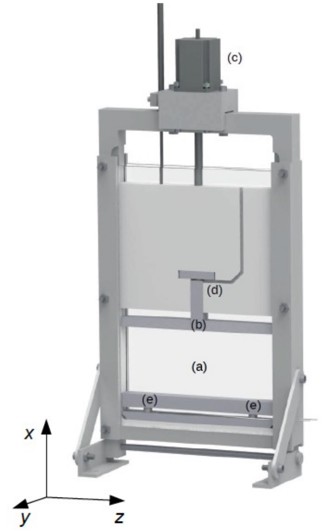
Experimental evidence of cross-diffusion waves in snow

- A cohesive aggregate of ice granules with density ρ = 370 kg/m^3 and grain sizes ranging from 0.1 to about 0.5 mm (mean grain size $\xi \approx 0.2$ mm) is compressed in an oedometric device.
- The velocity of the soliton-like wave is 7 times the piston velocity (1.12 mm/s).
- It accelerates after reflection.
- It disperses after reflection.









Barraclough et al. (2017, Nat. Phys.)

https://doi.org/10.1038/nphys3966

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Summary

- We propose a thermodynamics-based approach capturing dynamic feedbacks including phase transition for a generic dual-continuum (porous) system.
- A new class of quasi-soliton waves is discovered in porous geomaterials based on theory and numerical experiments, supported by physical experiments.
- These waves nucleate as excitation waves due to incompatibility of the local processes with large scale constraints.
- The waves are found to precede macroscopic failure of the material (for simplicity here only studied for volumetric modes).
- The approach suggests a minimal set of equations fully described by dynamic reaction-diffusion coefficients.
- The onset of dynamic localization phenomena is found to be controlled through mutual feedbacks of network forming processes by both solid as well as the fluid components of the system.