

# EXTENSIONS OF SYMPLECTIC NUMERICAL METHODS FOR SIMULATIONS OF IRREVERSIBLE SYSTEMS

**Tamás FÜLÖP**



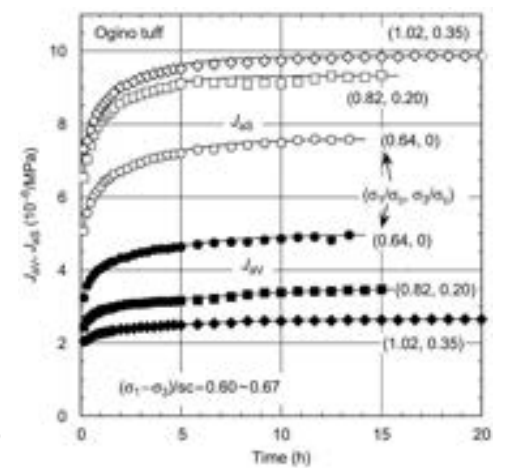
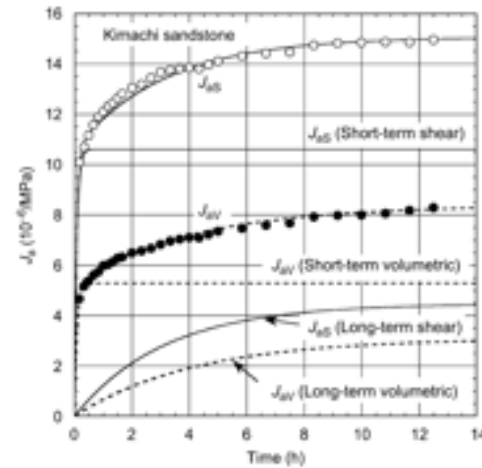
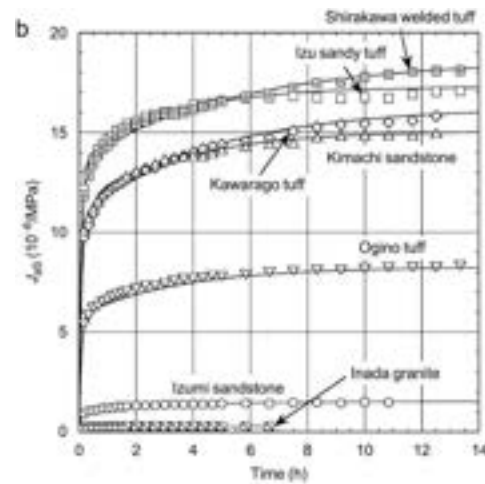
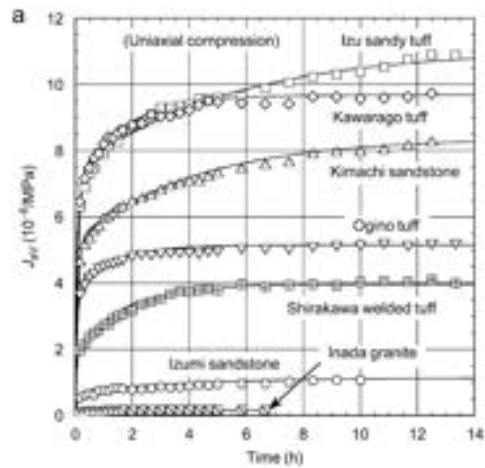
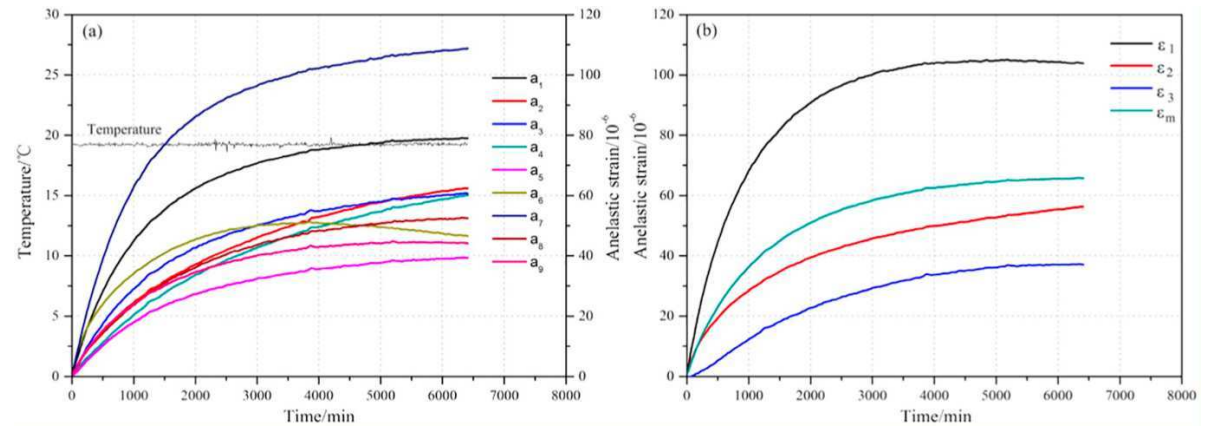
*Department of Energy Engineering,  
Budapest Univ. of Technology and Econ.*

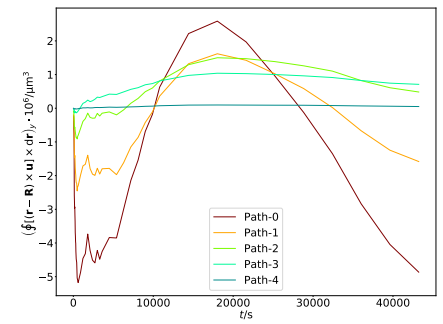
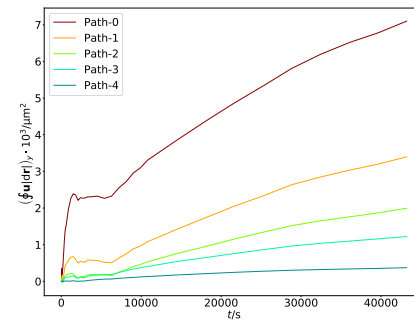
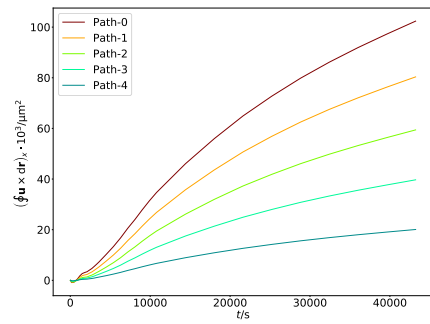
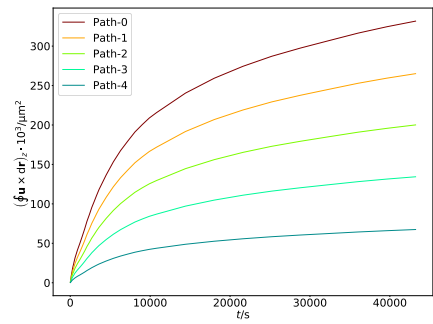
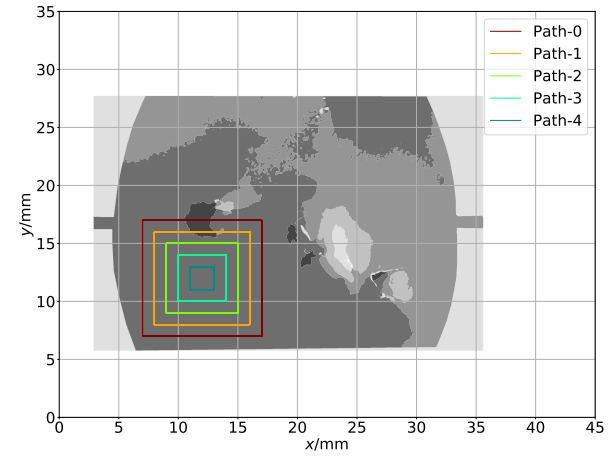
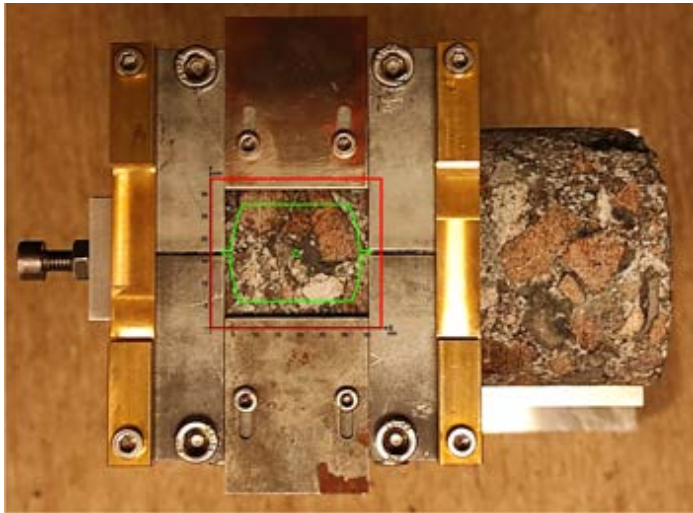
*Montavid Thermodynamic Research Group,  
Budapest, Hungary*



Miklós Farkas Seminar, BME, Budapest, 2024-02-22

# Motivations: Rocks





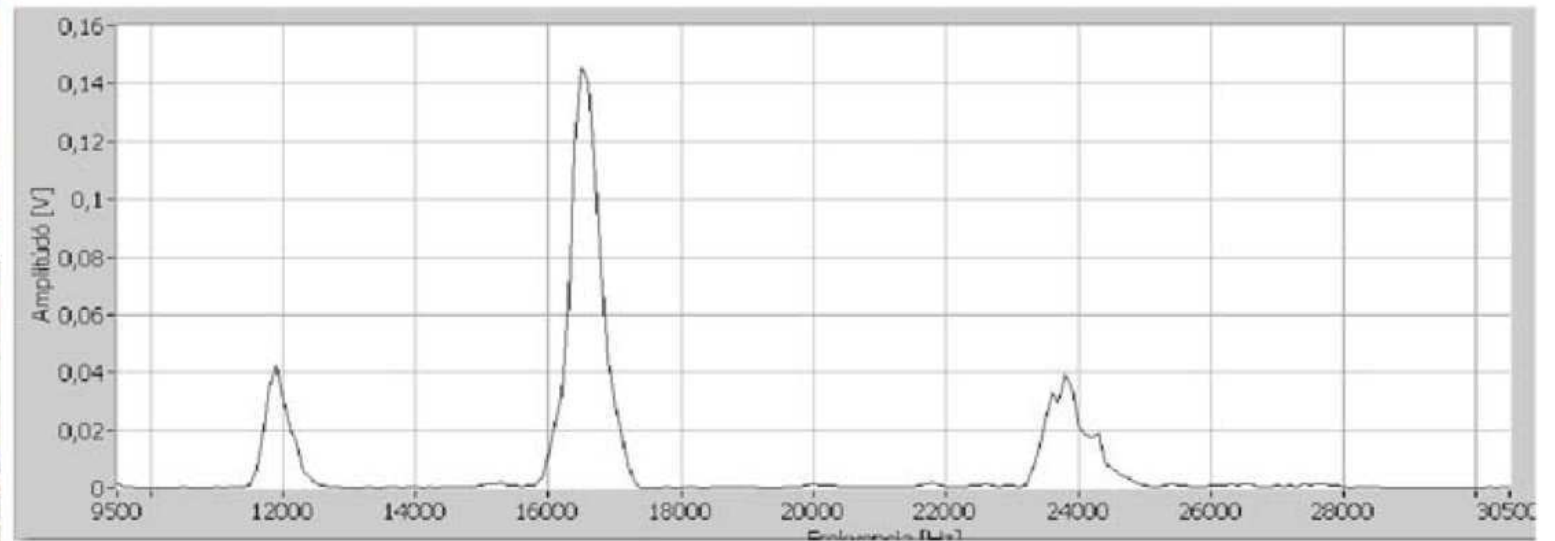
# Wave propagation:



MEGJEGYZÉS: Feltűl/alul apróhomokkő/finomhomokkő; T: 24,6 C° Relatív páratartalom: 57,50 %

MÉRÉSI ALAPADATOK:

Minta jele:	Származási hely [fm]:	Hossz [mm]:	Átmérő [mm]:	Tömeg [kg]:	Poisson tényező [-]:
FP-40-4T	Szolnok_Magraktár	51.85	37.90	0.1451	0.175

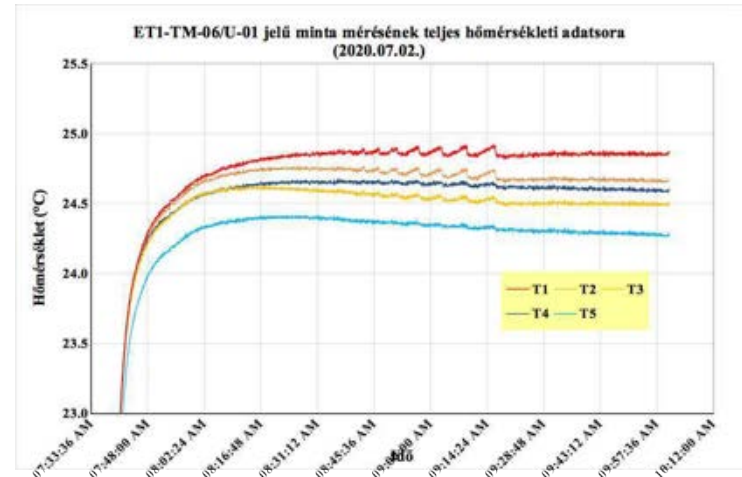
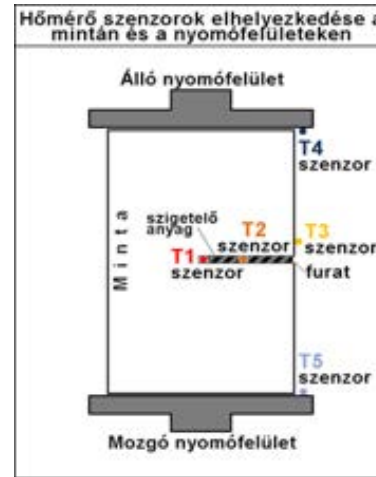
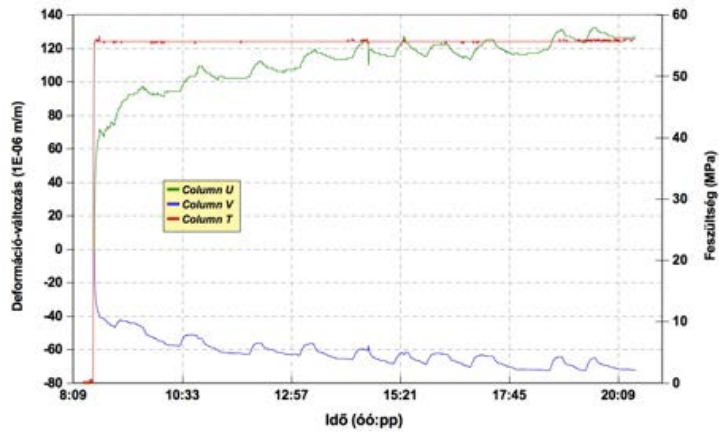


MÉRT ÉS SZÁMÍTOTT ÉRTÉKEK:

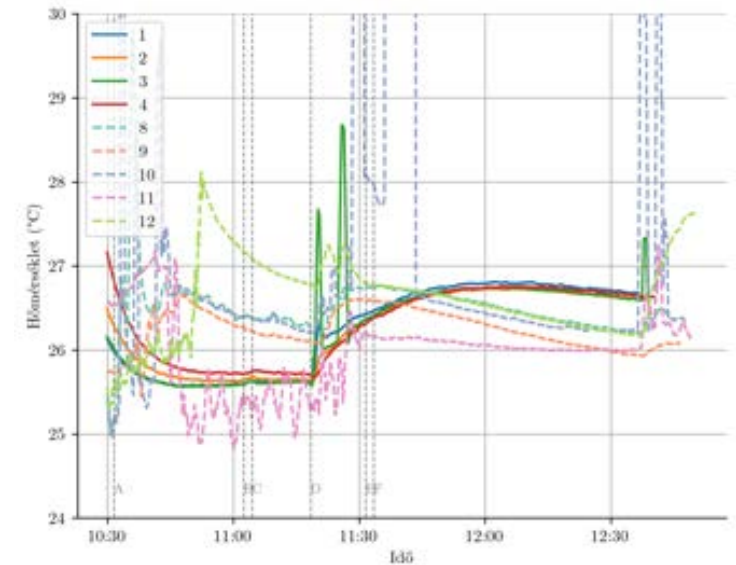
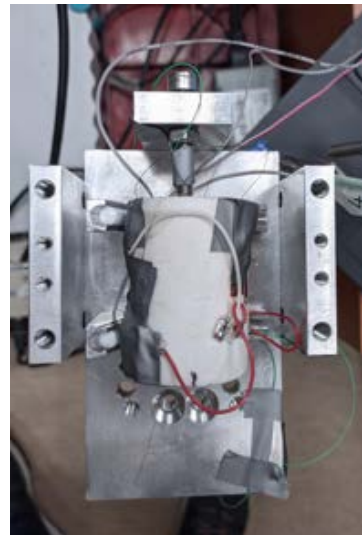
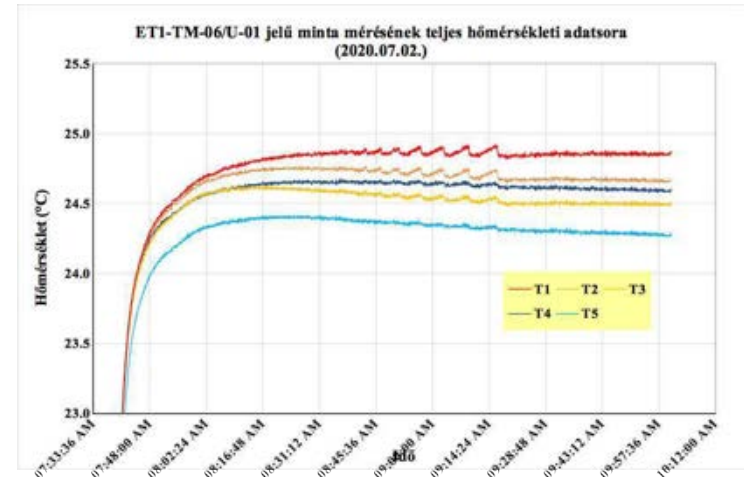
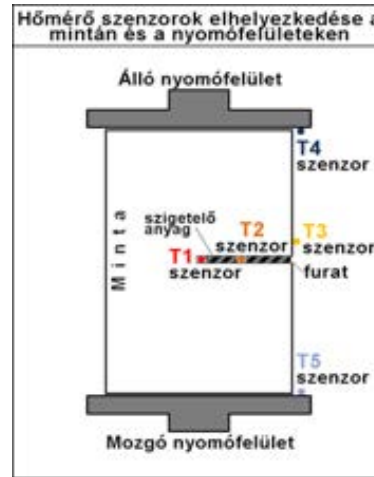
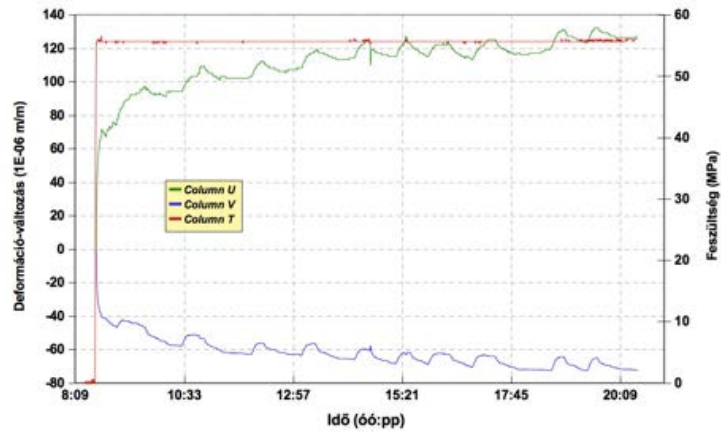
Térfogat [cm <sup>3</sup> ]:	Sűrűség [kg/m <sup>3</sup> ]:	Dilatációs rezonanciafrekvencia [Hz]:	Dilatációs rezgési sebesség [m/s]:	Dinamikus Young-modulus [GPa]:	Dinamikus nyírási modulus [GPa]:
58.49	2480.56	16500	1701.15	7.11	3.02



# Temperature: thermal expansion, heat conduction:



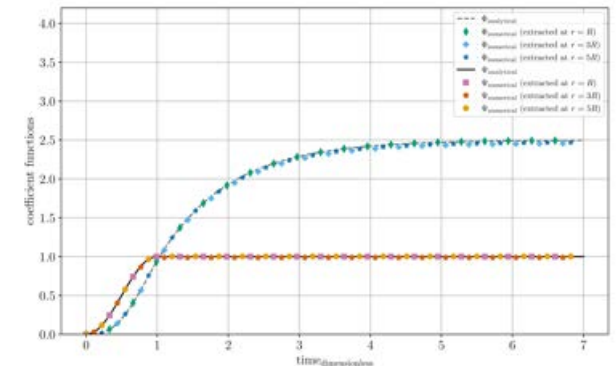
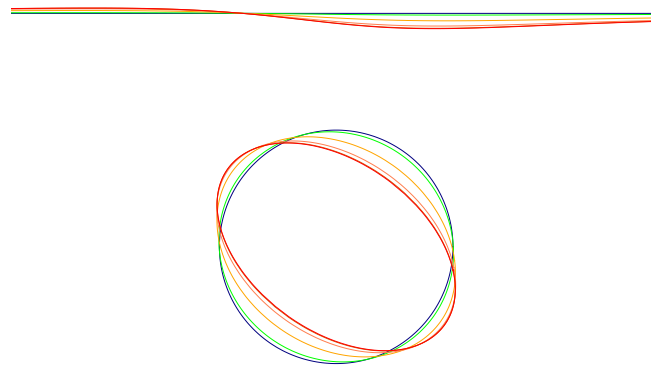
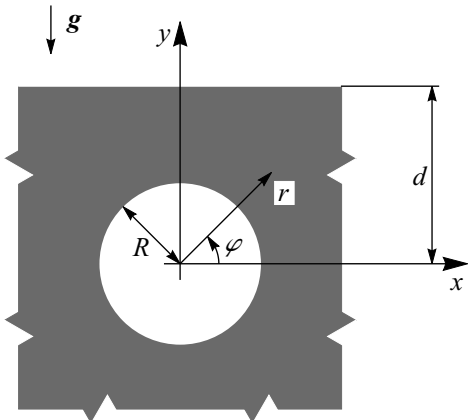
# Temperature: thermal expansion, heat conduction:



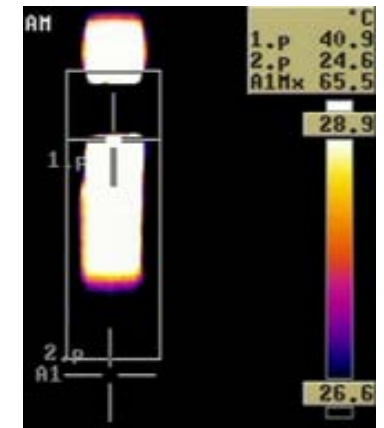
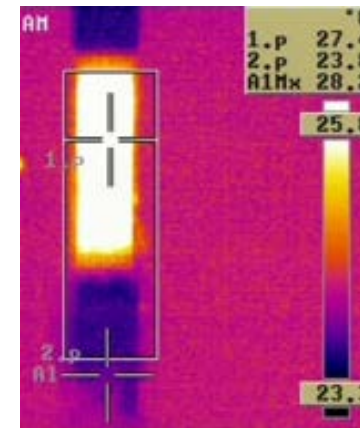
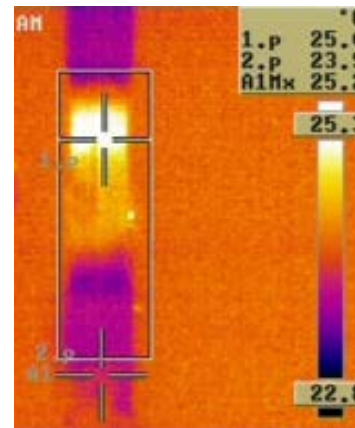
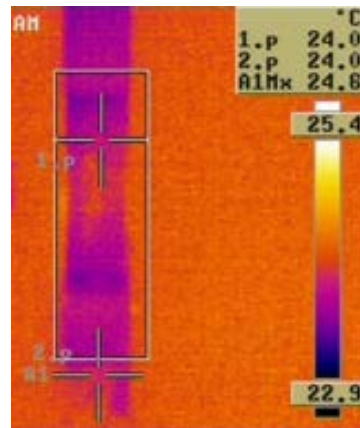
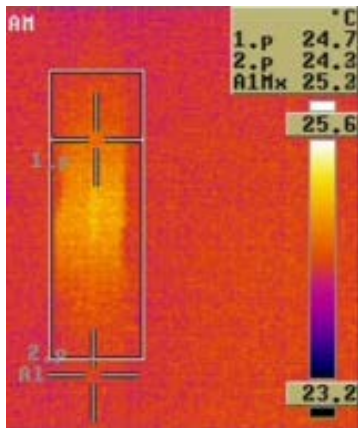
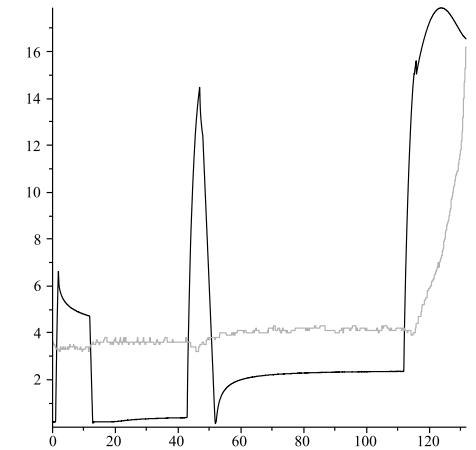
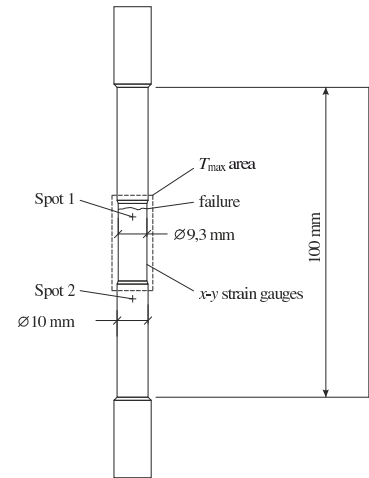
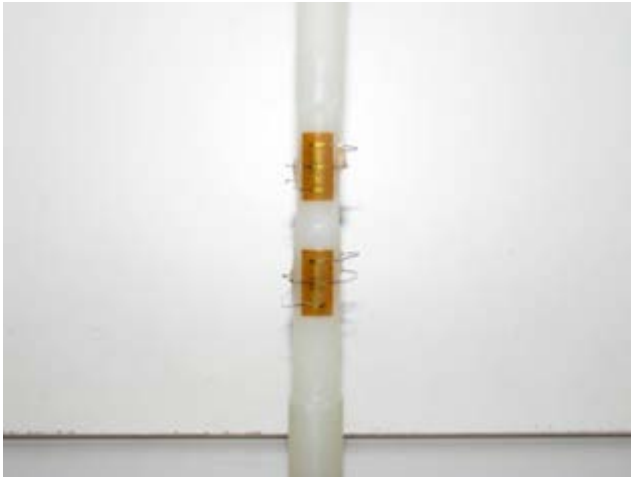
# Motivations: Tunnels: an analytical solution method:

$$\mathcal{L}^{\text{dev}} \sum_{k=1}^J \left[ \lambda_k(t) \sum_{j=1}^J c_j(\eta_k) \mathbf{s}_j^{\text{dev}}(\mathbf{r}) \right] = \mathcal{Z}^{\text{dev}} \sum_{k=1}^J \left[ \kappa_k(t) \sum_{j=1}^J \frac{1}{\eta_k} c_j(\eta_k) \mathbf{s}_j^{\text{dev}}(\mathbf{r}) \right]$$

$$\mathcal{L}^{\text{sph}} \sum_{k=1}^J \left[ \lambda_k(t) \sum_{j=1}^J c_j(\eta_k) \mathbf{s}_j^{\text{sph}}(\mathbf{r}) \right] = \mathcal{Z}^{\text{sph}} \sum_{k=1}^J \left[ \kappa_k(t) \sum_{j=1}^J c_j(\eta_k) \mathbf{s}_j^{\text{sph}}(\mathbf{r}) \right]$$



# Motivations: Plastics:

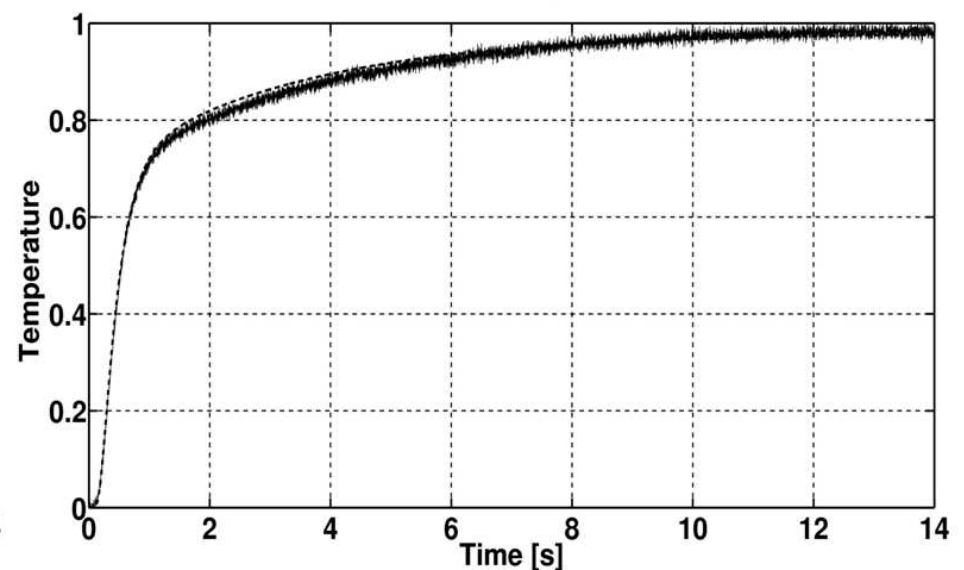
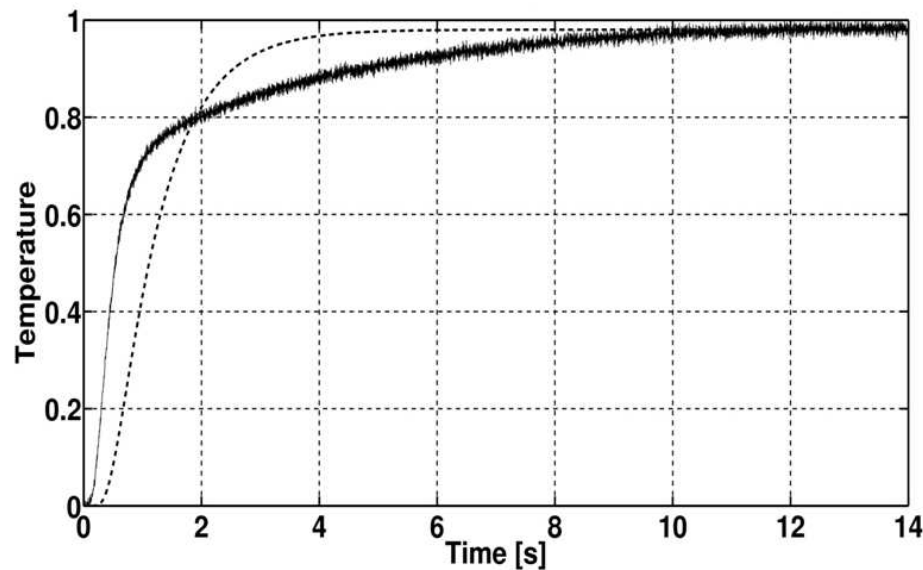
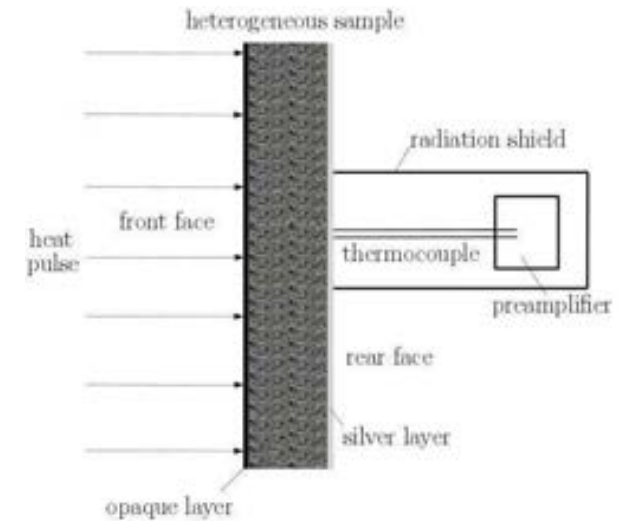




**Motivations:** Large-deformation elasticity + thermal expansion  
+ plasticity: compatibility criterion:

$$\begin{aligned}
& \text{tr}_{1,5;3,4} \left[ \mathbf{A}^{-1} \otimes \mathbf{A}^{-1} (\mathbf{A} \otimes \nabla) (\mathbf{A} \otimes \nabla) \right] + 2\mathbf{A}^{-1} \text{tr}_{1,2} [\mathbf{A} (\nabla \otimes \nabla \otimes \mathbf{A})] \mathbf{A}^{-1} \\
& \quad + 2\text{tr}_{2,3} \left[ \mathbf{A}^{-1} \otimes (\nabla \cdot \mathbf{A}) (\nabla \otimes \mathbf{A}) \right] \mathbf{A}^{-1} + 2\text{tr}_{1,2} \left[ \mathbf{A}^{-1} (\mathbf{A} \otimes \nabla \otimes \nabla) \right] \\
& \quad - 2\mathbf{A}^{-1} \text{tr}_{2,4} [(\mathbf{A} \otimes \nabla \otimes \nabla)] + 2\text{tr}_{1,4;3,5} \left[ \mathbf{A}^{-1} \otimes \mathbf{A}^{-1} (\mathbf{A} \otimes \nabla) (\mathbf{A} \otimes \nabla) \right] \\
& \quad \quad + \text{tr}_{1,2;3,5} \left[ \mathbf{A}^{-1} (\mathbf{A} \otimes \nabla) (\mathbf{A} \otimes \nabla) \otimes \mathbf{A}^{-1} \right] \\
& \quad - 2\mathbf{A}^{-1} \text{tr}_{2,5;3,6} \left[ (\mathbf{A} \otimes \nabla) \mathbf{A} (\nabla \otimes \mathbf{A}) \otimes \mathbf{A}^{-1} \right] \mathbf{A}^{-1} - 2[\nabla \otimes (\nabla \cdot \mathbf{A})] \mathbf{A}^{-1} \\
& + 2\text{tr}_{2,4} \left[ (\nabla \otimes \mathbf{A}) \mathbf{A}^{-1} (\mathbf{A} \otimes \nabla) \right] \mathbf{A}^{-1} - 3\text{tr}_{2,6;3,5} \left[ (\nabla \otimes \mathbf{A}) \mathbf{A}^{-1} (\mathbf{A} \otimes \nabla) \otimes \mathbf{A}^{-1} \right] \\
& \quad - \text{tr}_{3,4;2,5} \left[ \mathbf{A}^{-1} \otimes \mathbf{A}^{-1} (\mathbf{A} \otimes \nabla) \mathbf{A} (\nabla \otimes \mathbf{A}) \right] \mathbf{A}^{-1} \\
& \quad \quad - 2\mathbf{A}^{-1} \text{tr}_{2,4;3,5} [(\mathbf{A} \otimes \nabla) \otimes (\nabla \otimes \mathbf{A})] \mathbf{A}^{-1} = \mathbf{0}
\end{aligned}$$

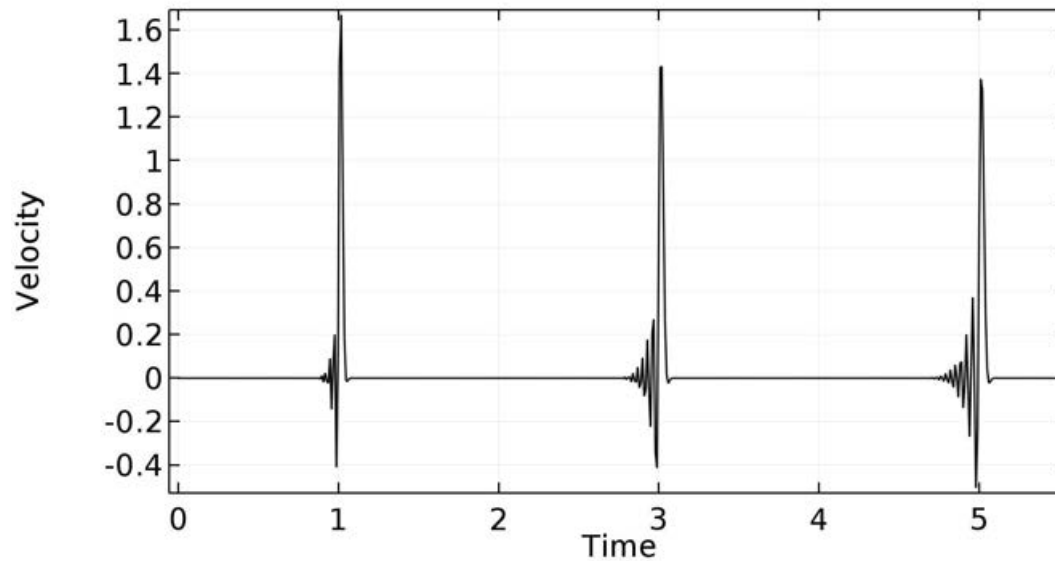
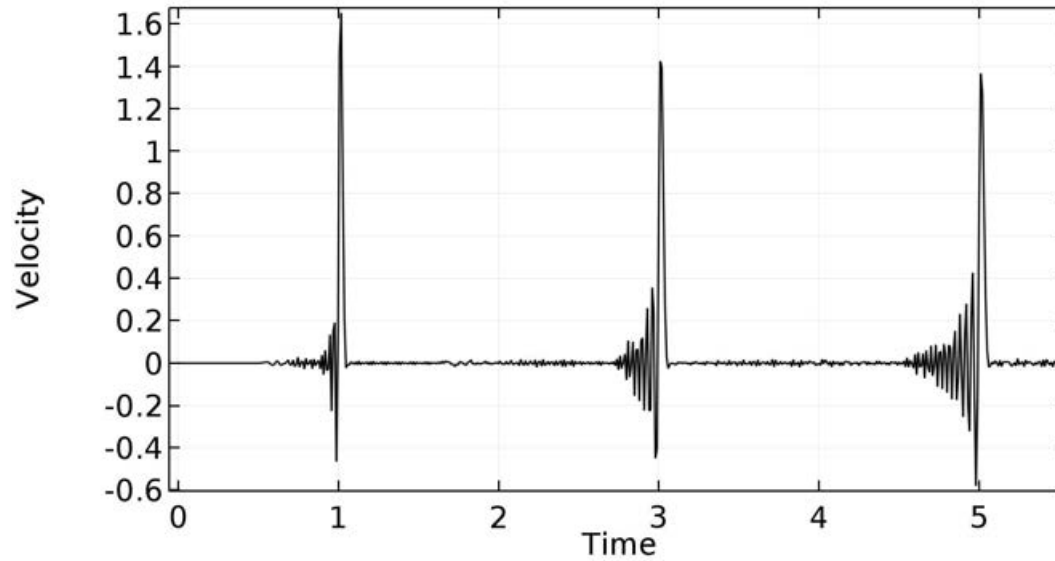
# Motivations: Beyond-Fourier heat conduction:



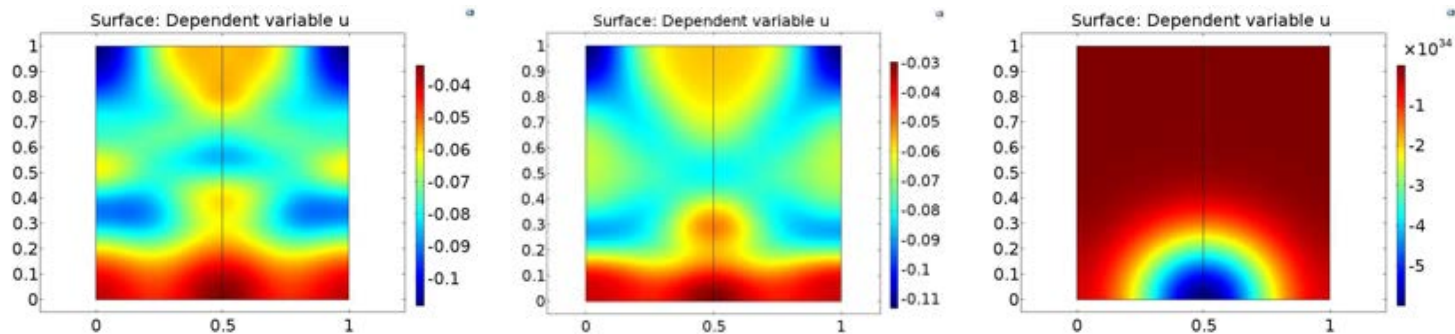
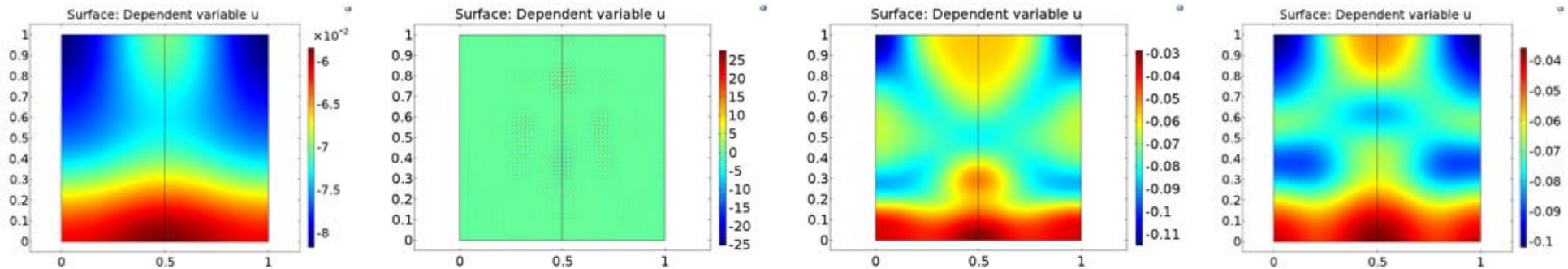
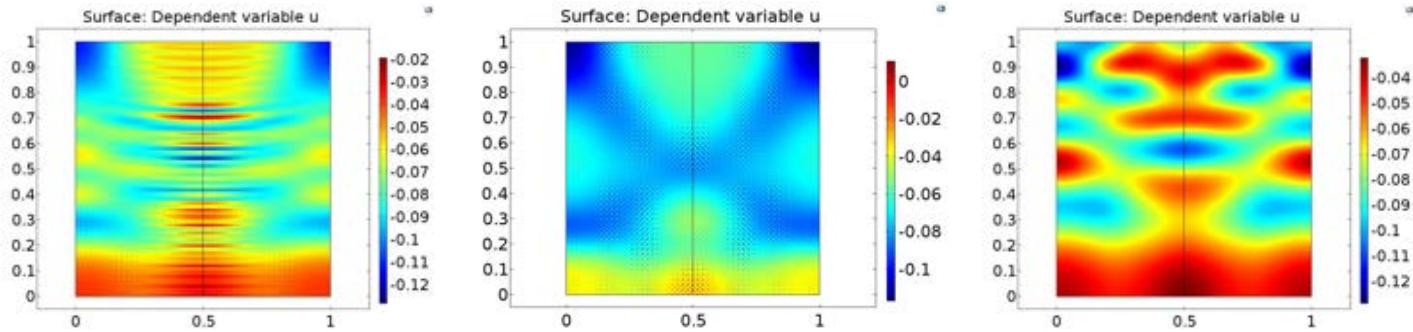
$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2}$$

$$\frac{\partial T}{\partial t} + \tau \frac{\partial^2 T}{\partial t^2} = a \frac{\partial^2 T}{\partial x^2} + b \frac{\partial^3 T}{\partial t \partial x^2}$$

# Commercial software: 1D wave propagation



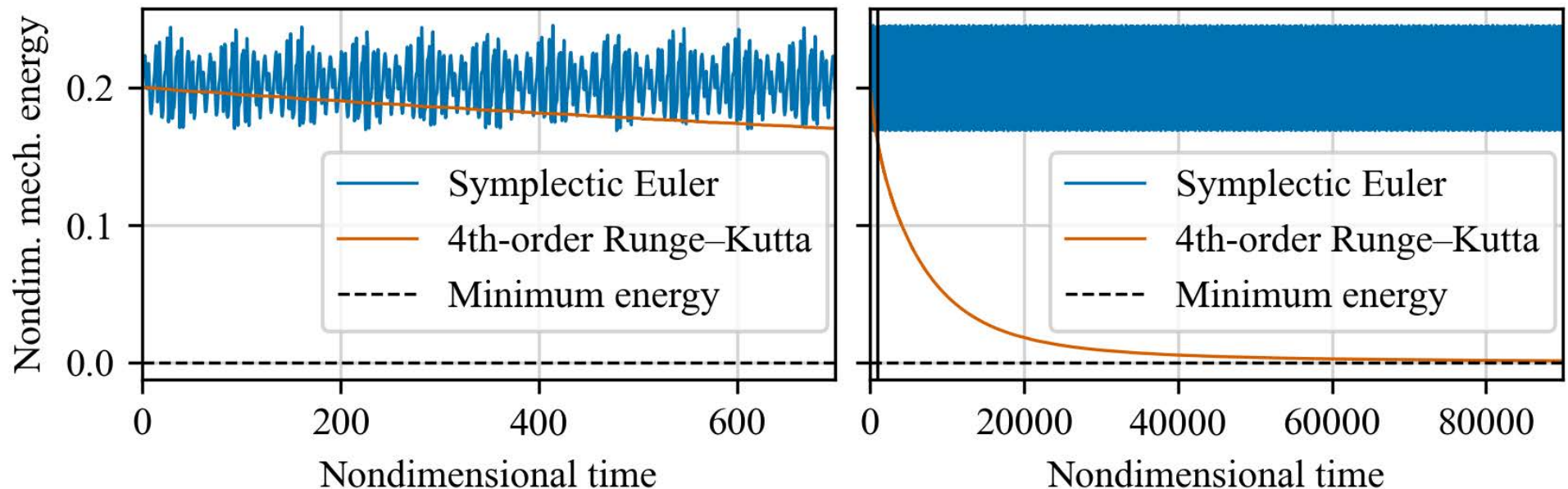
# Commercial software: 2D wave propagation



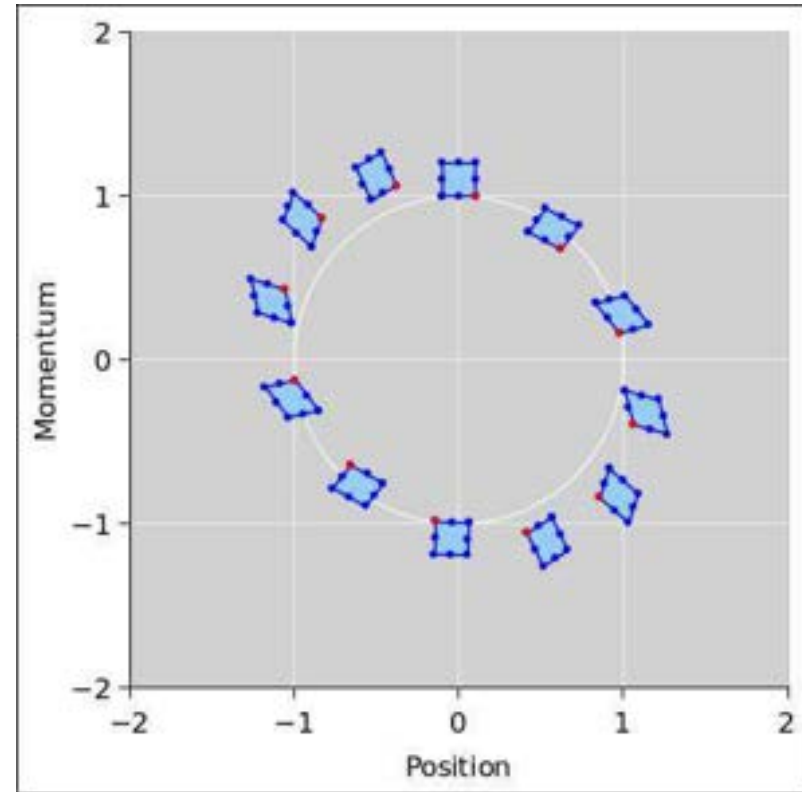
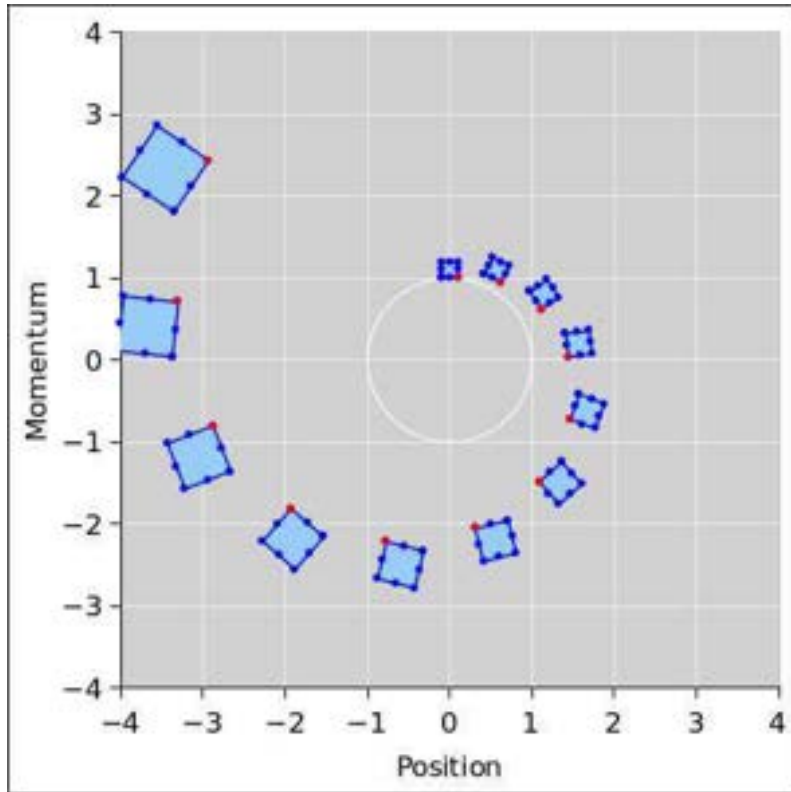
## Self-developed numerical schemes: structure-preserving

e.g., symplectic methods and irreversible extensions

On the example of the planar elastic pendulum:



# Nonsymplectic vs. symplectic in phase space: [J. Denker]



## Symplectic Euler: (1st-order accurate)

$$p_{n+1} = p_n - hH_q(p_{n+1}, q_n)$$

$$q_{n+1} = q_n + hH_p(p_{n+1}, q_n)$$

$$p_{n+1} = p_n - hH_q(p_n, q_{n+1})$$

$$q_{n+1} = q_n + hH_p(p_n, q_{n+1})$$

## Störmer–Verlet: (2nd-order accurate)

$$p_{n+1/2} = p_n - \frac{h}{2}H_q(p_{n+1/2}, q_n)$$

$$q_{n+1} = q_n + \frac{h}{2} \left( H_p(p_{n+1/2}, q_n) + H_p(p_{n+1/2}, q_{n+1}) \right)$$

$$p_{n+1} = p_{n+1/2} - \frac{h}{2}H_q(p_{n+1/2}, q_{n+1})$$

$$q_{n+1/2} = q_n + \frac{h}{2}H_q(p_n, q_{n+1/2})$$

$$p_{n+1} = p_n - \frac{h}{2} \left( H_p(p_n, q_{n+1/2}) + H_p(p_{n+1}, q_{n+1/2}) \right)$$

$$q_{n+1} = q_{n+1/2} + \frac{h}{2}H_q(p_{n+1}, q_{n+1/2})$$

**Structure-preserving:** *e.g.*,

symplectic (preserving a 2-form)

preserving energy, momentum, angular momentum etc.

variational

**Tools:** *e.g.*,

backward error analysis

modified vector field:  $\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z}(t)) \rightarrow \tilde{\mathbf{z}}(t+h) = \Phi_h(\tilde{\mathbf{z}}(t)) : \frac{d\tilde{\mathbf{z}}}{dt} = \tilde{\mathbf{f}}(\tilde{\mathbf{z}}(t))$

shadowing:  $\mathbf{z}(t_0) \rightarrow \hat{\mathbf{z}}(t_0)$



**Literature:** *e.g.*,

G Benettin, A Giorgilli (1994) *J. Stat. Phys.* 74, 1117

C Kane, JE Marsden, M Ortiz, M West (2000) *Int. J. Numer. Methods Eng.* 49, 1295

WB Hayes, KR Jackson (2003) *SIAM J. Numer. Anal.* 41, 1948

PC Moan (2006) *Journal of Physics A* 39, 5545

E Hairer, C Lubich, G Wanner (2006) *Geometric numerical integration*, Springer, Berlin

X Shang, HC Öttinger (2020) *Proc. R. Soc. A: Math. Phys. Eng. Sci.* 476, 20190446

## **Own works:**

T Fülöp, R Kovács, M Szücs, M Fawaiier: Thermodynamical extension of a symplectic numerical scheme with half space and time shifts demonstrated on rheological waves in solids, *Entropy* 22 (2020) 155

Á Pozsár, M Szücs, R Kovács, T Fülöp: Four spacetime dimensional simulation of rheological waves in solids and the merits of thermodynamics, *Entropy* 22 (2020) 1376

T Fülöp: Wave Propagation in Rocks – Investigating the Effect of Rheology, *Periodica Polytechnica Civil Engineering* 65 (2021) 26

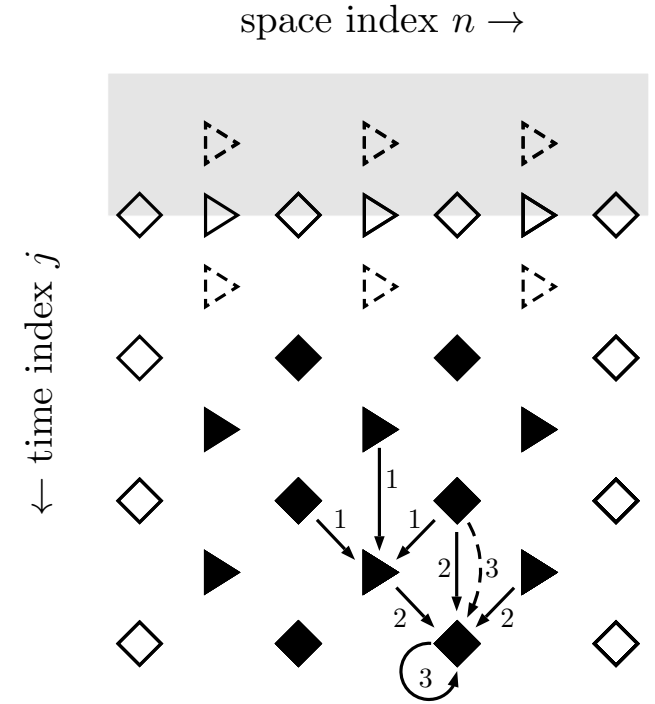
DM Takács, Á Pozsár, T Fülöp: Thermodynamically extended symplectic numerical simulation of viscoelastic, thermal expansion and heat conduction phenomena in solids, *Continuum Mech. Thermodyn.*, Early access (2024) DOI:10.1007/s00161-024-01280-w

DM Takács, T Fülöp: Improving the accuracy of the Newmark method through backward error analysis, submitted;  
DOI:10.48550/arXiv.2403.02029

$$\rho \frac{\partial v}{\partial t} = \frac{\partial \sigma}{\partial x}$$

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial v}{\partial x}$$

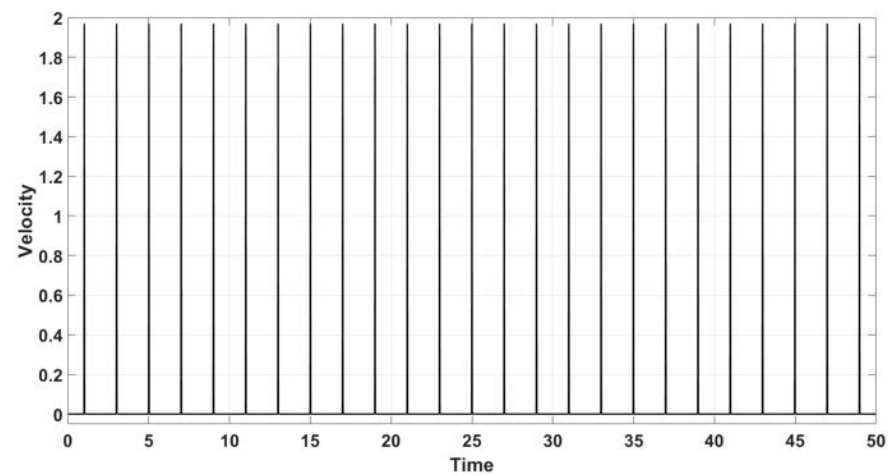
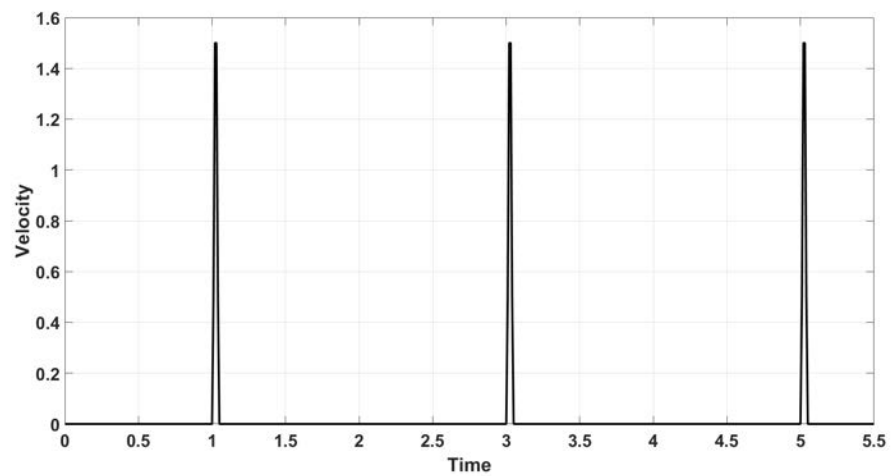
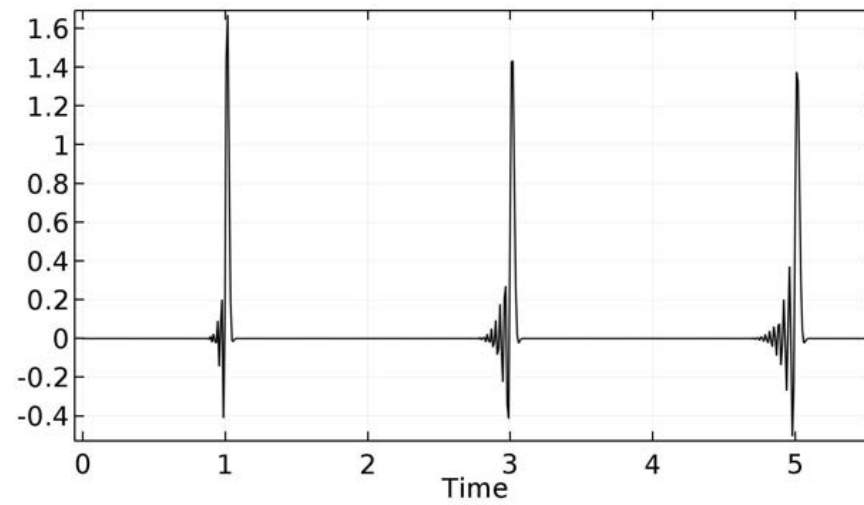
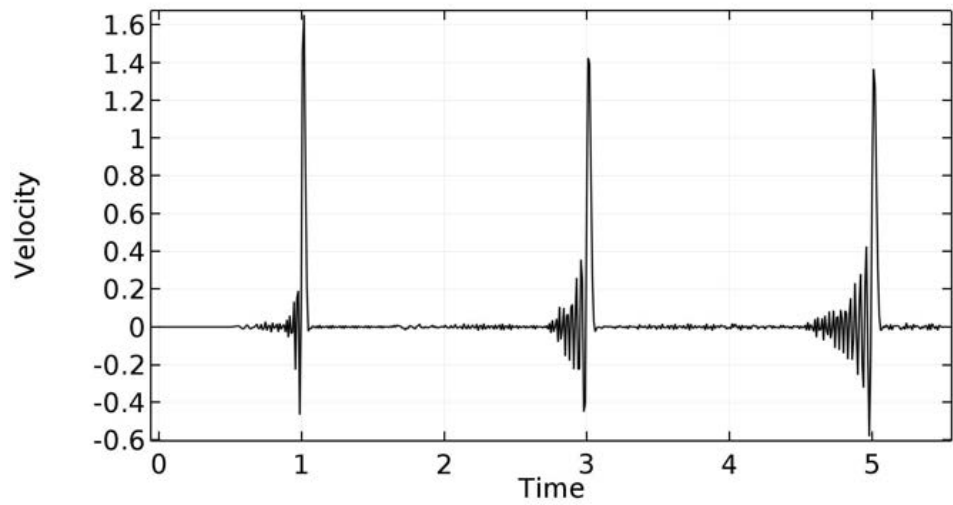
$$\sigma + \tau \frac{\partial \sigma}{\partial t} = E\varepsilon + \hat{E} \frac{\partial \varepsilon}{\partial t}$$



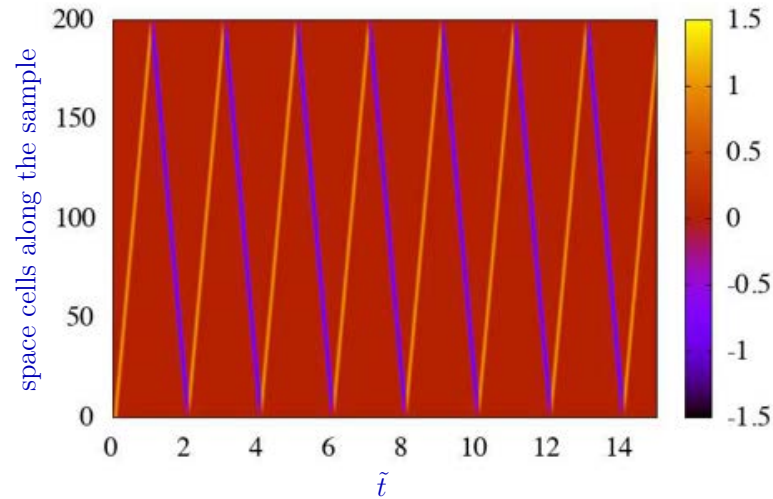
$$\rho \frac{v_{n+1/2}^{j+1/2} - v_{n+1/2}^{j-1/2}}{\Delta t} = \frac{\sigma_{n+1}^j - \sigma_n^j}{\Delta x}$$

$$\frac{\varepsilon_n^{j+1} - \varepsilon_n^j}{\Delta t} = \frac{v_{n+1/2}^{j+1/2} - v_{n-1/2}^{j+1/2}}{\Delta x}$$

$$\sigma_n^{j+1} = \frac{1}{1 - \alpha + \frac{\tau}{\Delta t}} \left\{ \left( \frac{\tau}{\Delta t} - \alpha \right) \sigma_n^j + E \left[ \alpha \varepsilon_n^j + (1 - \alpha) \varepsilon_n^{j+1} \right] + \hat{E} \frac{\varepsilon_n^{j+1} - \varepsilon_n^j}{\Delta t} \right\}$$

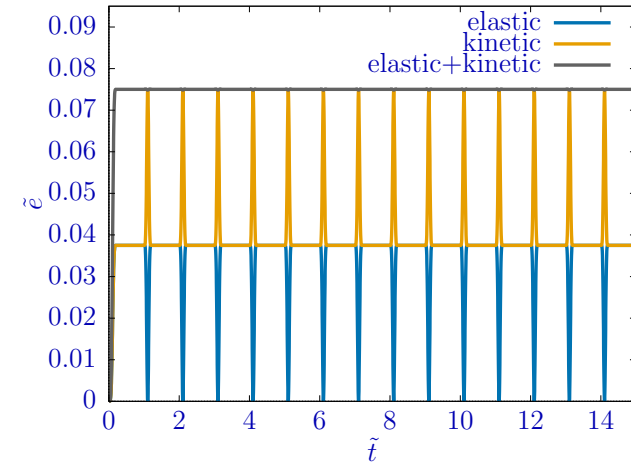


spacetime picture:

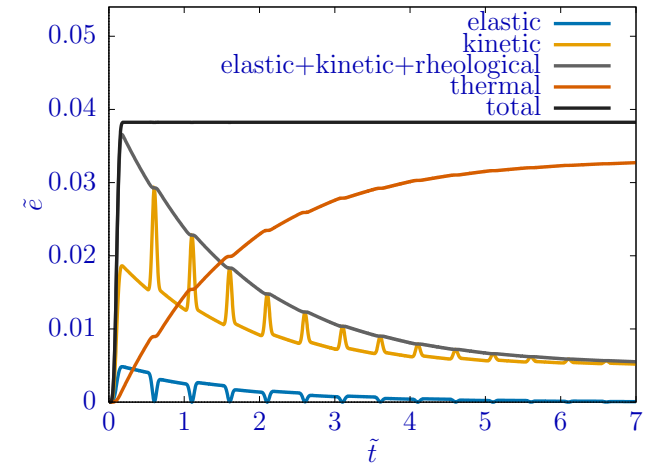
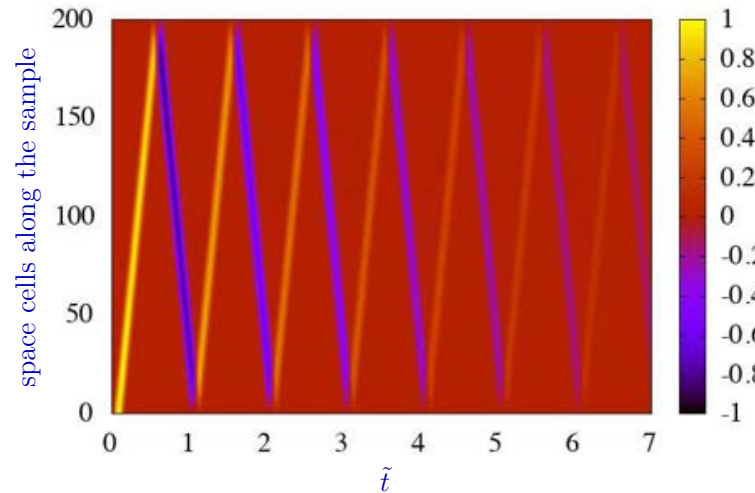


Hooke case:

time dependence  
of energies:

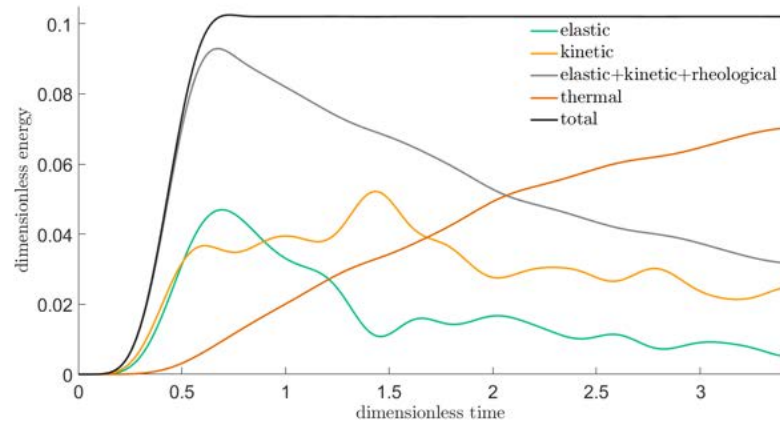
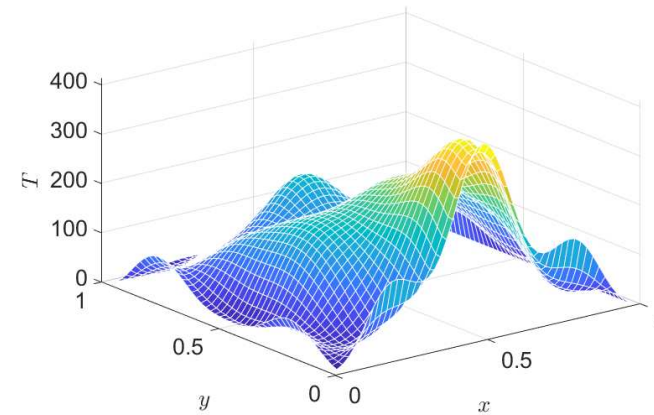
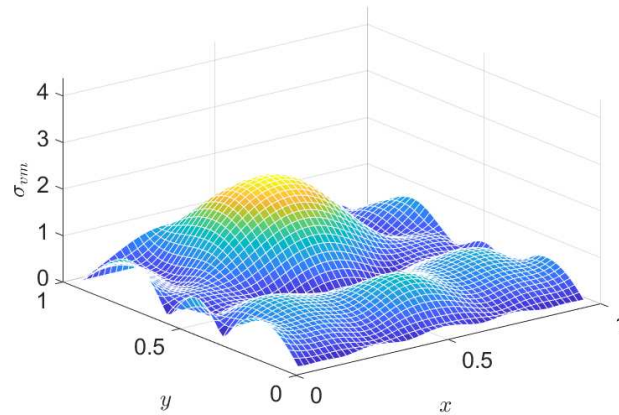
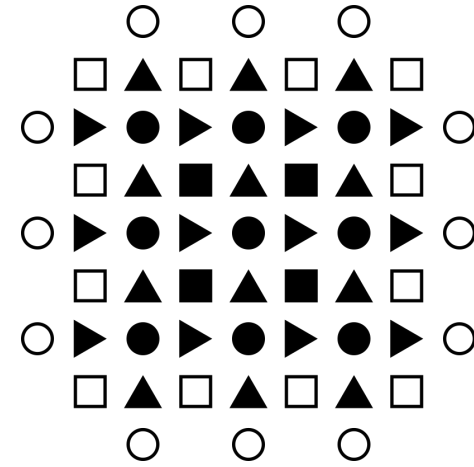


rheological  
case:



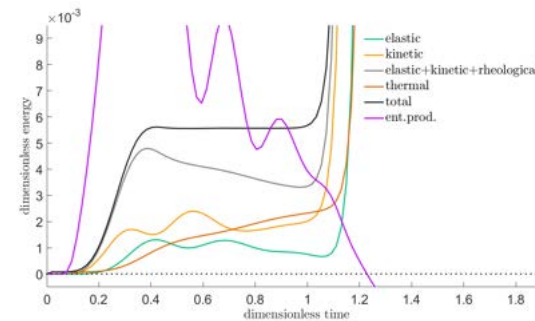
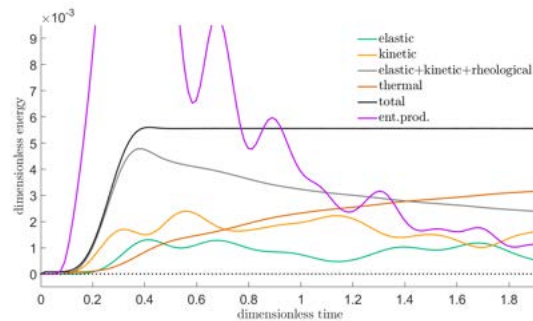
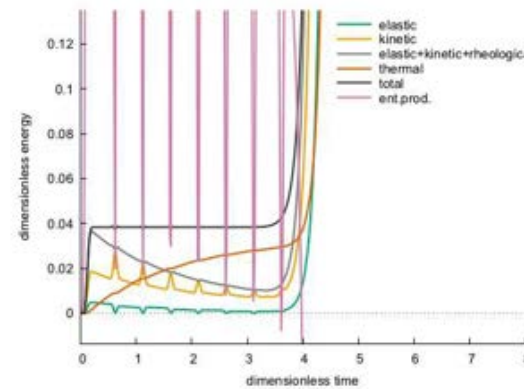
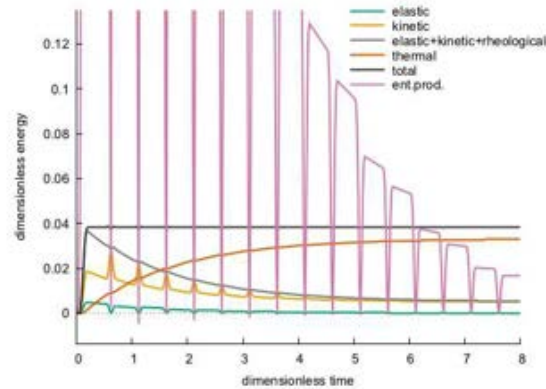
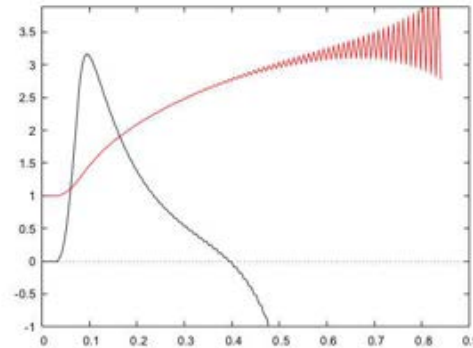
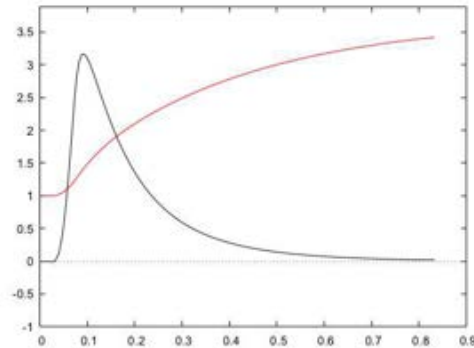
2 and 3 space dimensions:

different vector/tensor components:  
centers, faces, edges, vertices



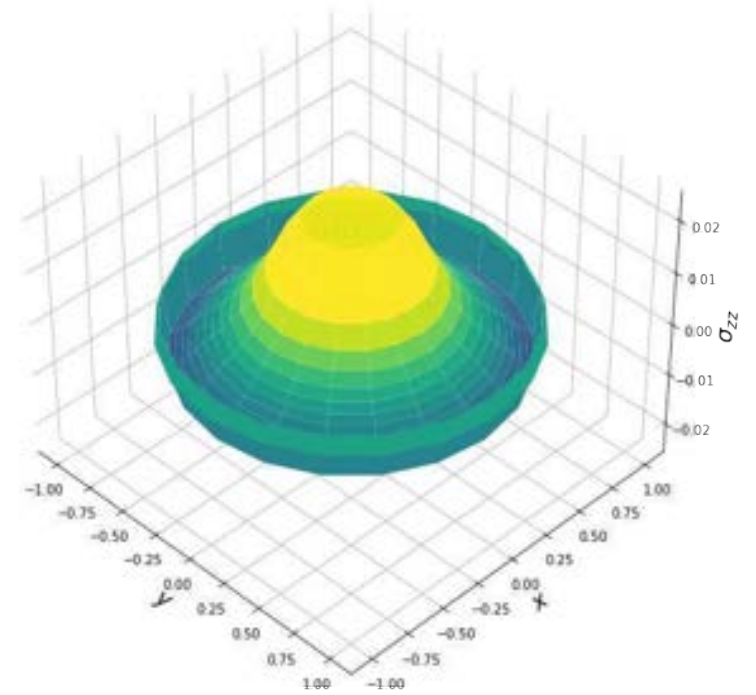
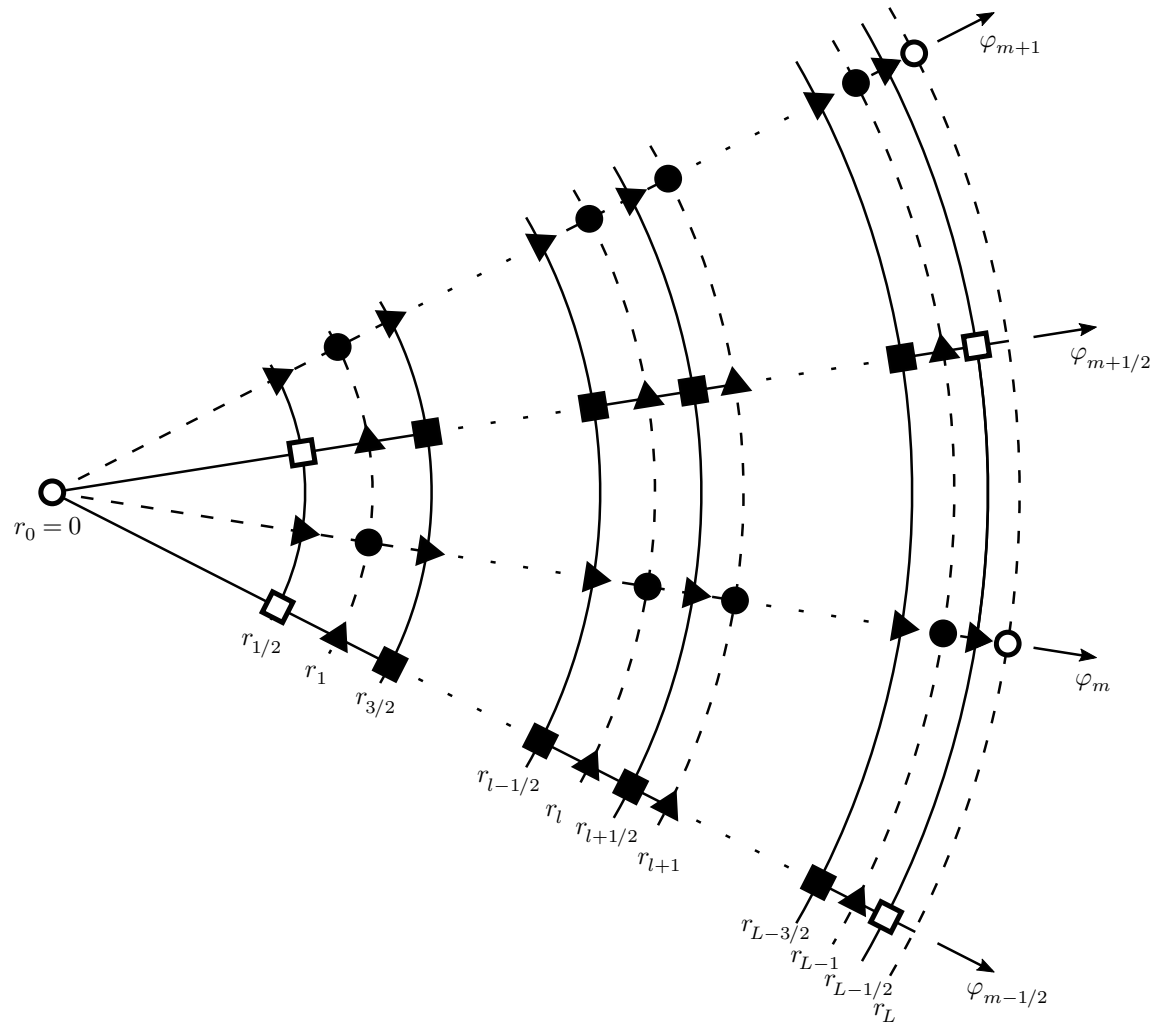
movie

# Entropy production rate: discretizing a „raw”, not automatically non-negative, form of it:





# Cylindrical geometry:



$$\rho \dot{v} = \frac{\partial \sigma}{\partial x} \quad (1)$$

$$\dot{\epsilon} = \frac{\partial v}{\partial x} \quad (2)$$

$$\sigma = \sigma_{\text{el}} + \hat{\sigma} \quad (3)$$

$$\hat{\sigma} + \tau \dot{\hat{\sigma}} = \hat{l} \dot{\epsilon} \quad (4)$$

$$\sigma_{\text{el}} = ED \quad (5)$$

$$e_{\text{int}} = e_{\text{thermal}} + e_{\text{elastic}} + e_{\text{rheol}} \quad (6)$$

$$\rho \dot{e}_{\text{int}} = -\frac{\partial q}{\partial x} + \sigma \dot{\epsilon} \quad (7)$$

$$\rho \dot{s} = -\frac{\partial \frac{q}{T}}{\partial x} + \underbrace{\frac{\partial \frac{1}{T}}{\partial x} q + \frac{\hat{\sigma}}{T} \left( \dot{\epsilon} - \frac{\tau}{\hat{l}} \dot{\hat{\sigma}} \right)}_{\pi_s} \quad (8)$$

$$q = -\lambda \frac{\partial T}{\partial x} \quad (9)$$

$$D = \epsilon - \alpha(T - T_{\text{ex}}) \quad (10)$$

$$e_{\text{total}} = \underbrace{\frac{v^2}{2}}_{e_{\text{kinetic}}} + \underbrace{c_{\text{ex}}(T - T_{\text{ex}})}_{e_{\text{thermal}}} + \underbrace{\frac{E}{2\rho} \epsilon(\epsilon + \alpha T_{\text{ex}})}_{e_{\text{elastic}}} + \underbrace{\frac{\tau}{2\rho \hat{l}} \hat{\sigma}^2}_{e_{\text{rheol}}} \quad (11)$$

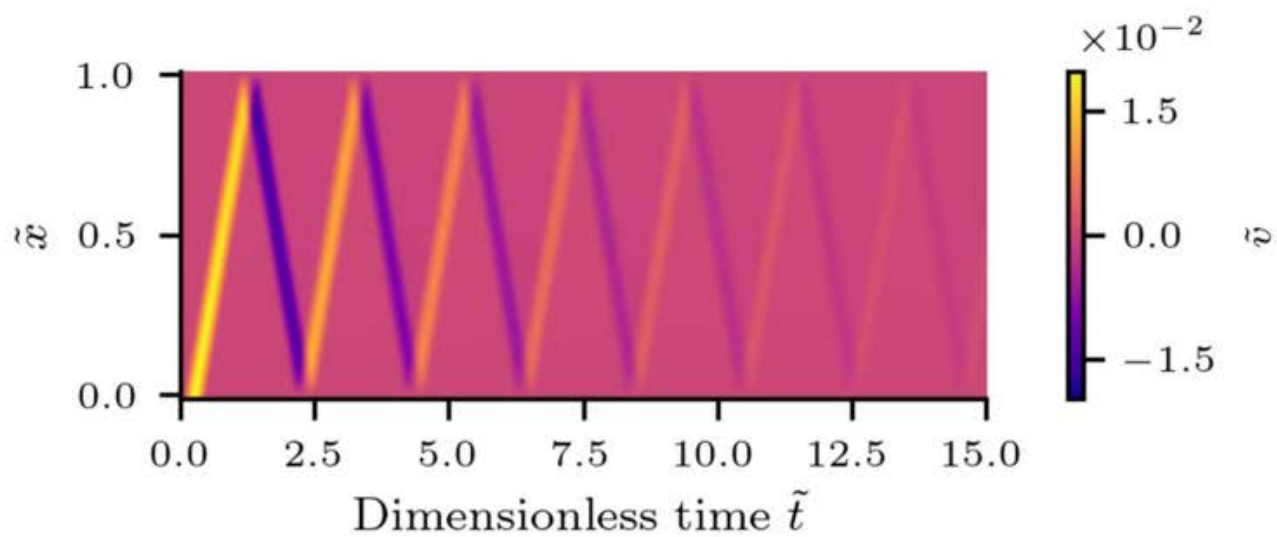


$$\begin{aligned}
v_{n+1/2}^{j+1/2} &\stackrel{(1)}{=} v_{n+1/2}^{j-1/2} + \frac{1}{\rho} \frac{\Delta t}{\Delta x} (\sigma_{n+1}^j - \sigma_n^j), \\
L_n^{j+1/2} &\stackrel{(3)}{=} \frac{1}{\Delta x} (v_{n+1/2}^{j+1/2} - v_{n-1/2}^{j+1/2}), \\
L_n^j &= \frac{1}{2} (L_n^{j+1/2} + L_n^{j-1/2}), \\
e_n^{j+1} &\stackrel{(13)}{=} e_n^j + \Delta t L_n^{j+1/2}, \\
e_n^{j+1/2} &= \frac{1}{2} (e_n^{j+1} + e_n^j), \\
\hat{\sigma}_n^{j+1} &\stackrel{(4)}{=} \frac{1}{\frac{\tau}{\Delta t} + \frac{1}{2}} \left[ \hat{I} L_n^{j+1/2} + \left( \frac{\tau}{\Delta t} - \frac{1}{2} \right) \hat{\sigma}_n^j \right], \\
\hat{\sigma}_n^{j+1/2} &= \frac{1}{2} (\hat{\sigma}_n^{j+1} + \hat{\sigma}_n^j); \tag{17}
\end{aligned}$$

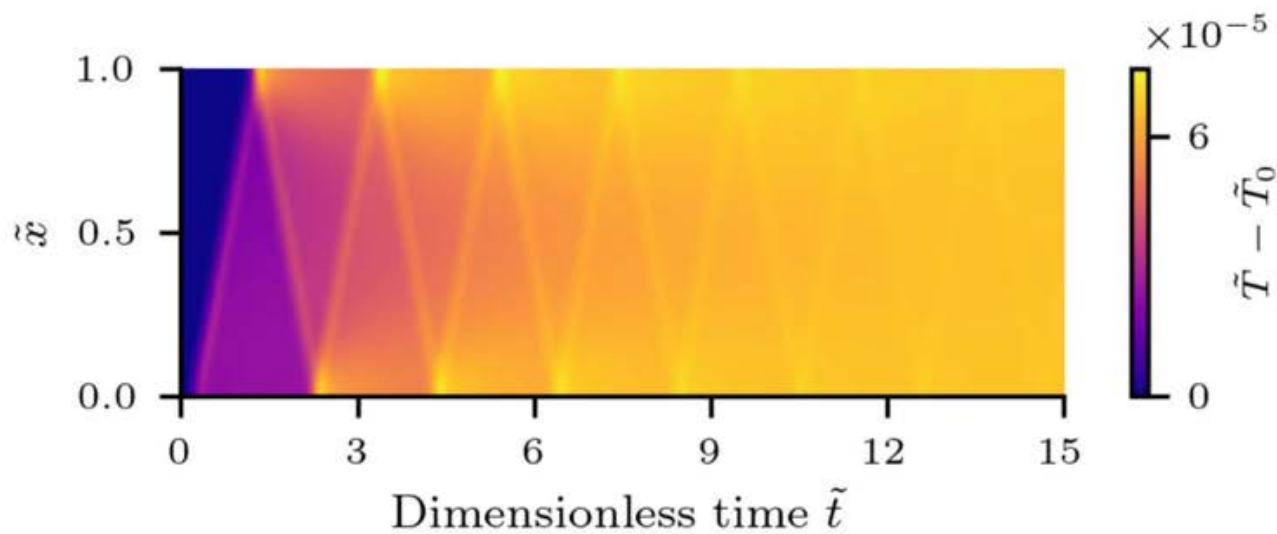
$$\begin{aligned}
(e_{\text{int}})_n^{j+1/2} &\stackrel{(11)}{=} (e_{\text{int}})_n^{j-1/2} - \frac{1}{\rho} \frac{\Delta t}{\Delta x} [(j_e)_{n+1/2}^j - (j_e)_{n-1/2}^j] + \frac{\Delta t}{\rho} \sigma_n^j L_n^j, \\
T_n^{j+1/2} &\stackrel{(6)}{=} T_{\text{ex}} + \frac{1}{c_{\text{ex}}} \left[ (e_{\text{int}})_n^{j+1/2} - \frac{E}{2\rho} e_n^{j+1/2} (e_n^{j+1/2} + 2\alpha T_{\text{ex}}) \right. \\
&\quad \left. - \frac{\tau}{2\rho \hat{I}} (\hat{\sigma}_n^{j+1/2})^2 \right],
\end{aligned}$$

$$\begin{aligned}
(j_e)_{n+1/2}^{j+1/2} &\stackrel{(8)}{=} -\frac{\lambda}{\Delta x} (T_{n+1}^{j+1/2} - T_n^{j+1/2}), \\
D_n^{j+1/2} &\stackrel{(14)}{=} e_n^{j+1/2} - \alpha (T_n^{j+1/2} - T_{\text{ex}}), \\
(\sigma_{\text{el}})_n^{j+1/2} &\stackrel{(15)}{=} E D_n^{j+1/2}, \\
\sigma_n^{j+1/2} &\stackrel{(2)}{=} (\sigma_{\text{el}})_n^{j+1/2} + \hat{\sigma}_n^{j+1/2}; \tag{18} \\
(e_{\text{int}})_n^{j+1} &\stackrel{(11)}{=} (e_{\text{int}})_n^j - \frac{1}{\rho} \frac{\Delta t}{\Delta x} \left\{ \left[ 2(j_e)_{n+1/2}^j - (j_e)_{n+1/2}^{j-1/2} \right] \right. \\
&\quad \left. - \left[ 2(j_e)_{n-1/2}^j - (j_e)_{n-1/2}^{j-1/2} \right] \right\} + \frac{\Delta t}{\rho} \sigma_n^{j+1/2} L_n^{j+1/2}, \\
T_n^{j+1} &\stackrel{(6)}{=} T_{\text{ex}} + \frac{1}{c_{\text{ex}}} \left[ (e_{\text{int}})_n^{j+1} - \frac{E}{2\rho} e_n^{j+1} (e_n^{j+1} + 2\alpha T_{\text{ex}}) - \frac{\tau}{2\rho \hat{I}} (\hat{\sigma}_n^{j+1})^2 \right], \\
(j_e)_{n+1/2}^{j+1} &\stackrel{(8)}{=} -\frac{\lambda}{\Delta x} (T_{n+1}^{j+1} - T_n^{j+1}), \\
D_n^{j+1} &\stackrel{(14)}{=} e_n^{j+1} - \alpha (T_n^{j+1} - T_{\text{ex}}), \\
(\sigma_{\text{el}})_n^{j+1} &\stackrel{(15)}{=} E D_n^{j+1}, \\
\sigma_n^{j+1} &\stackrel{(2)}{=} (\sigma_{\text{el}})_n^{j+1} + \hat{\sigma}_n^{j+1}. \tag{19}
\end{aligned}$$

Velocity:

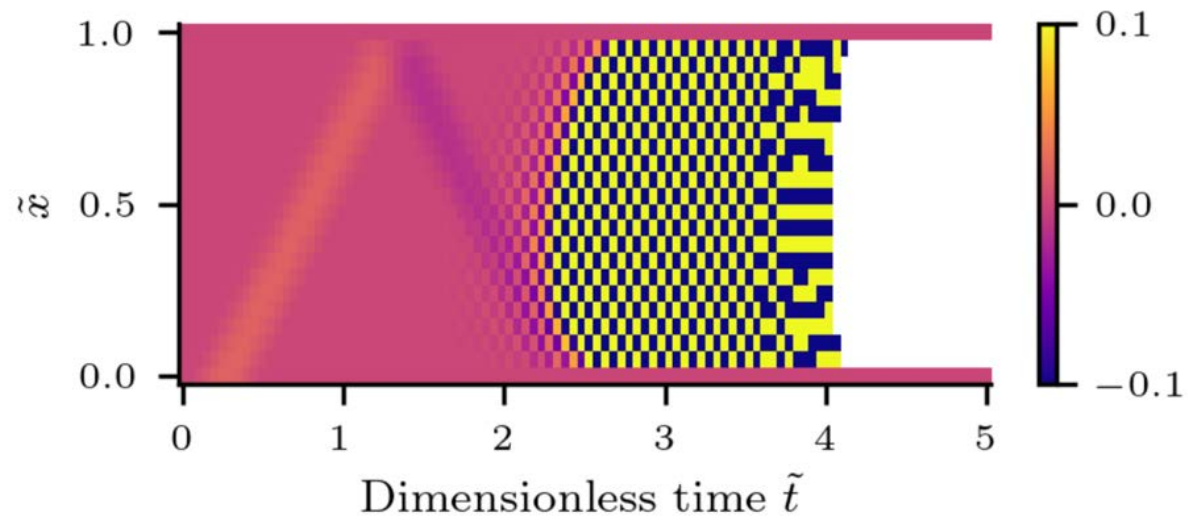


Temperature:



## Loss of stability:

Velocity:



Conclusions:

symplectic and other structure-preserving schemes:

Conclusions:

symplectic and other structure-preserving schemes:

- direct realizations and extensions



Conclusions:

symplectic and other structure-preserving schemes:

- direct realizations and extensions
- heuristic extensions (inspiration)

Conclusions:

symplectic and other structure-preserving schemes:

- direct realizations and extensions
- heuristic extensions (inspiration)

benefits of not eliminating degrees of freedom

Conclusions:

symplectic and other structure-preserving schemes:

- direct realizations and extensions
- heuristic extensions (inspiration)

benefits of not eliminating degrees of freedom

benefits of quantities with a balance law

Conclusions:

symplectic and other structure-preserving schemes:

- direct realizations and extensions
- heuristic extensions (inspiration)

benefits of not eliminating degrees of freedom

benefits of quantities with a balance law

benefits of the spacetime view

Conclusions:

symplectic and other structure-preserving schemes:

- direct realizations and extensions
- heuristic extensions (inspiration)

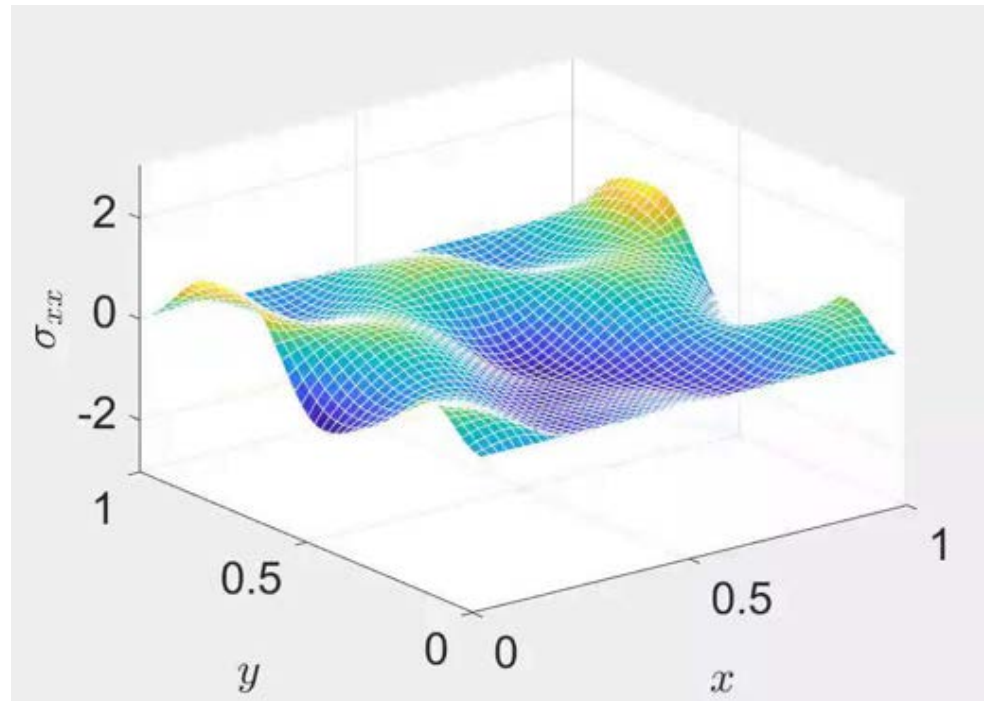
benefits of not eliminating degrees of freedom

benefits of quantities with a balance law

benefits of the spacetime view

benefits of strong mathematical results

THANK YOU FOR YOUR ATTENTION!



+ thanks to my co-authors

Róbert Kovács, Mátyás Szücs, Áron Pozsár, Donát M. Takács  
(alphabetic order)