Symmetry Methods in mechanics of materials and rheology

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Outline

- Thermodynamic approach of relaxation and time-temperature superposition principle from Lie symmetries (direct approach)

- Inverse modeling approach: constitutive laws from Lie groups as a general strategy

- Example: acrylic polymer stickes under low velocity impact

- Outlook

A thermodynamic approach of relaxation

Basic assumption :

"The Gibbs relation is valid for situations outside equilibrium"

$$dE = \boldsymbol{\sigma} : d(V\boldsymbol{\varepsilon}) + TdS + \mu dN \qquad \text{Gibbs relation}$$

$$V\boldsymbol{\varepsilon} : d\boldsymbol{\sigma} + SdT + Nd\mu = 0 \qquad \text{Gibbs-Duhem relation}$$

→ Internal energy potential $E = E(\boldsymbol{y}, \boldsymbol{z})$

$\boldsymbol{y}$: extensive controlled variables $\rightsquigarrow (s, \boldsymbol{\gamma})$

$\boldsymbol{z}$: extensive internal variables (microstructure)

→ Extensity property $\quad E(\lambda \boldsymbol{y}, \lambda \boldsymbol{z}) = \lambda E(\boldsymbol{y}, \boldsymbol{z})$ (Callen)

Euler relation

$$E = \frac{\partial E}{\partial \boldsymbol{y}} \cdot \boldsymbol{y} + \frac{\partial E}{\partial \boldsymbol{z}} \cdot \boldsymbol{z}$$

→

- Intensive observable variables $\quad \boldsymbol{Y} = \dfrac{\partial E}{\partial \boldsymbol{y}}$
- Generalized non equilibrium forces $\quad \boldsymbol{A} = -\dfrac{\partial E}{\partial \boldsymbol{z}}$

Thermodynamic framework of relaxation

$$dN_k = dN_k^e + dN_k^i$$

$$N_k^i = \sum_j \nu_{jk}\xi_j, \quad \xi_j \text{ degré d'avancement réaction chimique}$$

$$\begin{pmatrix} \dot{\boldsymbol{Y}} \\ -\dot{\boldsymbol{A}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{a^u} & \boldsymbol{b} \\ \boldsymbol{b^T} & \boldsymbol{g} \end{pmatrix} \begin{pmatrix} \dot{\boldsymbol{y}} \\ \dot{\boldsymbol{z}} \end{pmatrix}$$

Thermodynamic information

$$\boldsymbol{a^u} = \frac{\partial^2 E}{\partial \boldsymbol{y}^2}$$

Tisza matrix

$$\boldsymbol{g} = \frac{\partial^2 E}{\partial \boldsymbol{z}^2}$$

Dissipation matrix

$$\boldsymbol{b} = \frac{\partial^2 E}{\partial \boldsymbol{y}\partial \boldsymbol{z}}$$

Coupling matrix

$\Leftrightarrow$

Maxwell relations for E

$$\frac{\partial^2 E}{\partial x_i \partial x_j} = \frac{\partial^2 E}{\partial x_j \partial x_i}$$

(where $\boldsymbol{x} = \boldsymbol{y}$ or $\boldsymbol{z}$)

$\rightarrow$

E remains a thermodynamic potential during the evolution

Kinetic equations for the internal variables

$\boldsymbol{z}$: non controlled variables outside equilibrium
(internal reorganizations)

→ Kinetics law $\boxed{\dot{\boldsymbol{z}} = \boldsymbol{L} \cdot \boldsymbol{A}}$ $L_{ij} = L_{ji}$ (Onsager's properties)

→ Relaxed state $\boxed{-\dot{\boldsymbol{A}}^{\boldsymbol{r}} = 0}$

$$-\dot{\boldsymbol{A}} = \boldsymbol{b}^{\boldsymbol{T}} \cdot \dot{\boldsymbol{y}} + \boldsymbol{g} \cdot \dot{\boldsymbol{z}} \quad \Rightarrow \quad \begin{cases} \dot{\boldsymbol{z}}^{r} = -\boldsymbol{g}^{-1} \cdot \boldsymbol{b}^{\boldsymbol{T}} \cdot \dot{\boldsymbol{y}} \\ \dot{\boldsymbol{z}} = -(\boldsymbol{L} \cdot \boldsymbol{g})(\boldsymbol{z} - \boldsymbol{z}^{\boldsymbol{r}}) \end{cases}$$

$\boxed{\boldsymbol{\tau} = (\boldsymbol{L} \cdot \boldsymbol{g})^{-1}}$

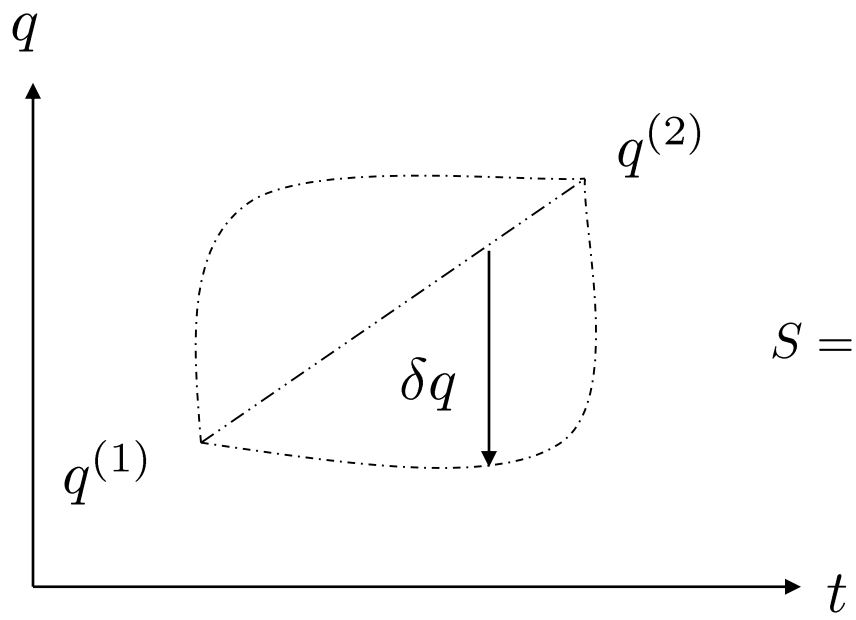
Relaxation time

→ Internal variables evolution (kinetic information)

$$\boxed{\dot{z}_k = -\frac{z_k - z_k^r}{\tau_k}}$$

Constitutive law and least action principle

Challenge : conciliate Hamiltonian dynamics with irreversible thermodynamics



$$S = \int_{t_1}^{t^2} dt \int_{\Omega_1} L d\Omega$$

PLA : $\delta S = 0$ with respect to the variations of the d.o.f. δq_i

$L = L((q_i, \dot{q}_i, \nabla q_i, \dots), i = 1 \dots N$ Lagrange density

$\rightarrow$ Euler-Lagrange equations (necessary conditions) :

$$-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \nabla.\left(\frac{\partial L}{\partial \nabla q_i}\right) + \frac{\partial L}{\partial q_i} = 0$$

Least action principle: historical perspective

- Helmholz : first attempts to reduce the principle of TIP to general principles of mechanics
- Onsager (1931) : principle of least dissipation or energy, cornerstone of modern TIP
- Gyarmati : integral principle of thermodynamics → force variation at constant fluxes combined with energy balance

Lagrange densities having arguments not being of the type $\{q, \dot{q}\}$

→ Euler-Lagrange equations $-\nabla.\left(\frac{\partial L}{\partial \nabla q_i}\right) + \frac{\partial L}{\partial q_i} = 0$ truncated from their temporal dimensions

→ Non-Hamiltonian action $S = \int_{\Omega_t} L d\Omega$

Lagrangian formulation of the constitutive laws

Constitutive law in rate form : $\mathbf{P} = \begin{cases} \boldsymbol{P}_Y(\boldsymbol{y},\boldsymbol{z}) = \dot{\boldsymbol{Y}} - \boldsymbol{e}_{,\mathrm{yy}}.\dot{\boldsymbol{y}} - \mathbf{e}_{,\mathrm{yz}}.\dot{\mathbf{z}} = 0 \\ \mathbf{P_A}(\boldsymbol{y},\boldsymbol{z}) = \dot{\mathbf{A}} - \mathbf{e}_{,\mathrm{zy}}.\dot{\mathbf{y}} - \mathbf{e}_{,\mathrm{zz}}.\dot{\mathbf{z}} = 0 \end{cases}$

Self-adjunction condition of the Frechet derivative of $\mathbf{P}$:

$$Dp = Dp^{\star} \rightarrow e_{,x_j x_i} = e_{,x_i x_j}, x \in \{\boldsymbol{y},\boldsymbol{z}\}$$

→ Maxwell conditions for internal energy satisfied due to its status of potential

→ Existence theorem of a Lagrangian [Santilli] :

$\mathbf{P}(\mathbf{u}) = \left\{\mathrm{P_i}\left(\mathbf{x},\mathbf{u}^{(\mathrm{n})}\right), \mathrm{i} = 1\ldots\mathrm{q}\right\}$ system of PDE's for the dependent variables $\mathbf{u}$.

System $\mathbf{P}(\mathbf{u}) = 0$ extremum of a functional integral $S = \int_\Omega L d\Omega$,

viz $P_i = E_i(L)$, iff $(Dp)_{ij} = (Dp^{\star})_{ij}$.

Possible Lagrangian $L = \int_0^1 \mathbf{u} P(\lambda\mathbf{u})\mathrm{d}\lambda = \int_0^1 \mathbf{u_i}\mathrm{P_i}(\lambda\mathbf{u})\mathrm{d}\lambda$

$\rightarrow L = \int_0^1 \left[\mathbf{y}.\mathbf{P}_{\mathrm{Y}}(\lambda\mathbf{y},\lambda\mathbf{z}) + \mathbf{z}.\mathbf{P}_{\mathrm{A}}(\lambda\mathbf{y},\lambda\mathbf{z})\right]$

Lagrangian formulation of the constitutive laws (2)

Account for extensity of order -1 of second derivatives of e :

$$e_{,yy}(\lambda y, \lambda z) = \frac{e_{,yy}(y,z)}{\lambda} \qquad e_{,yz}(\lambda y, \lambda z) = \frac{e_{,yz}(y,z)}{\lambda}$$
$$e_{,zy}(\lambda y, \lambda z) = \frac{e_{,zy}(y,z)}{\lambda} \qquad e_{,zz}(\lambda y, \lambda z) = \frac{e_{,zz}(z,z)}{\lambda}$$

and extensity order 0 of the intensive variables :

$$\mathbf{Y}(\lambda \mathbf{y}, \lambda \mathbf{z}) = \mathbf{Y}(\mathbf{y}, \mathbf{z})\,;\ \mathbf{A}(\lambda \mathbf{y}, \lambda \mathbf{z}) = \mathbf{A}(\mathbf{y}, \mathbf{z})$$

$$\rightarrow L = \mathbf{y}.\dot{\mathbf{Y}} - \mathbf{z}.\dot{\mathbf{A}} + \mathbf{e}_{,\mathrm{y}}.\dot{\mathbf{y}} + \mathbf{e}_{,\mathrm{z}}.\dot{\mathbf{z}} + \frac{\mathbf{d}}{\mathbf{dt}}\left(\mathbf{e}_{,\mathrm{y}}.\mathbf{y} + \mathbf{e}_{,\mathrm{z}}.\mathbf{z}\right)$$

Equivalent Lagrangian : the Euler-Lagrange equations are nil, viz $E_i(U) = 0, \forall i = 1 \ldots q$, iff U is the generalized divergence of a quadrivector $\mathbf{P}$:

$$Div\boldsymbol{P} = \sum_{i=1}^{4} \frac{dP_i}{dx_i} \equiv \frac{dP_t}{dt} + \frac{dP_x}{dx} + \frac{dP_y}{dy} + \frac{dP_z}{dz}$$

Lagrangian formulation of the constitutive laws (3)

$\rightarrow$ use Gibbs-Duhem relation : $\mathbf{y}.\dot{\mathbf{Y}} - \mathbf{z}.\dot{\mathbf{A}} = 0 \Rightarrow \mathrm{L} = \mathbf{e}_{,\mathrm{y}}\dot{\mathbf{y}} + \mathbf{e}_{,\mathrm{z}}\dot{\mathbf{z}} = \dfrac{\mathrm{de}(\mathbf{y},\mathbf{z})}{\mathrm{dt}}$

$\rightarrow$ Stationarity condition of the action integral $\delta S = \delta e = \delta \int_0^t \dfrac{de}{dt} dt = \delta \int_0^t de = 0$

Physical sense

internal energy keeps its status of a potential function during dynamic evolution.

Generalization of Poincaré lemma to functional forms [Olver, 1993] :

$\delta\omega = \int_\Omega [d\mathbf{u} \wedge (\mathbf{D}^*_{\mathbf{P}} - \mathbf{D}_{\mathbf{P}})]\mathbf{dx})$ $\qquad P = \{P_i(\mathbf{x}, \mathbf{u}^{(\mathbf{n})}), \mathbf{i} = \mathbf{1}..\mathbf{q}\}$

let one-form $\omega = \int_\Omega (\mathbf{P}.\mathbf{du})\mathbf{dx}$ $\qquad D_P$ Frechet derivative of $\mathbf{P}$

if ω is written in the form $\omega = \delta\psi$ with $\psi = \int_\Omega L(\mathbf{x}, \mathbf{u}^{(\mathbf{n})})\mathbf{dx}$

$\longrightarrow$ Get following equivalence : $\omega = \delta\psi = \delta \int_\Omega L(\mathbf{x}, \mathbf{u}^{(\mathbf{n})})\mathrm{dx} \Leftrightarrow \delta\omega = \delta\delta\psi = 0$

Form is exact equivalent to the fact that it is closed

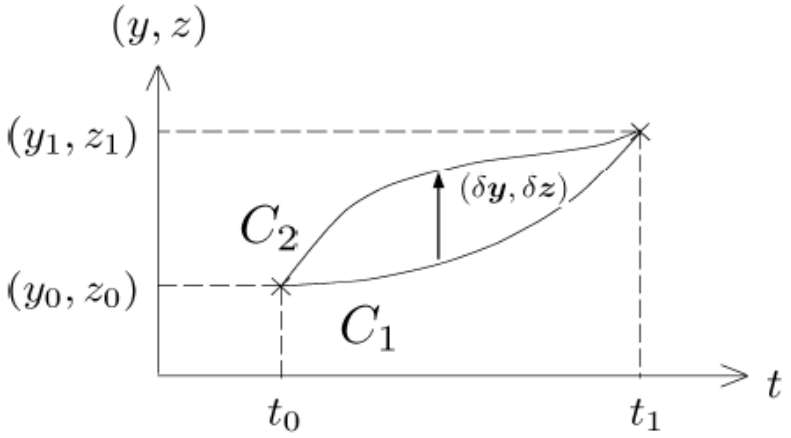
$$dd\psi = \sum_{1<i<j<q} \left(\frac{\partial^2\psi}{\partial u_i \partial u_j} - \frac{\partial^2\psi}{\partial u_j \partial u_i}\right) du_i \wedge du_j = 0 \Leftrightarrow \frac{\partial^2\psi}{\partial u_i \partial u_j} = \frac{\partial^2\psi}{\partial u_j \partial u_i}$$

$\longrightarrow$ Maxwell's conditions for the functional ψ

Lagrange formalism associated to the internal energy

$$\frac{\partial^2 E}{\partial x_i \partial x_j} = \frac{\partial^2 E}{\partial x_j \partial x_i}$$

(where $\boldsymbol{x} = \boldsymbol{y}$ or $\boldsymbol{z}$)



$$\int_{C_1} dE(\boldsymbol{y}, \boldsymbol{z}) = \int_{C_2} dE(\boldsymbol{y}, \boldsymbol{z})$$

$$\delta \int_{t_0}^{t_1} \dot{E} dt = 0$$

Lagrangian $L = \dot{E}$

$$\left.\begin{aligned} \frac{\partial \dot{E}}{\partial \boldsymbol{y}} - \frac{d}{dt}\left(\frac{\partial \dot{E}}{\partial \dot{\boldsymbol{y}}}\right) = 0 \\ \frac{\partial \dot{E}}{\partial \boldsymbol{z}} - \frac{d}{dt}\left(\frac{\partial \dot{E}}{\partial \dot{\boldsymbol{z}}}\right) = 0 \end{aligned}\right\} \Leftrightarrow \begin{pmatrix} \dot{\boldsymbol{Y}} \\ -\dot{\boldsymbol{A}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{a^u} & \boldsymbol{b} \\ \boldsymbol{b^T} & \boldsymbol{g} \end{pmatrix} \begin{pmatrix} \dot{\boldsymbol{y}} \\ \dot{\boldsymbol{z}} \end{pmatrix}$$

(Euler-Lagrange equations)

True for any thermodynamic potential (according to the choice of control variables)

Incorporation of the kinetics of internal variables

relations $\dot{z}_k = -\dfrac{z_k - z_k^r}{\tau_k}$ not contained in the lagrangian $L = \dot{\psi}$

→ considered as N constraints (N dissipative modes) $\displaystyle\int_{t_0}^{t_1} \left(\dot{z}_k + \frac{z_k - z_k^r}{\tau_k}\right) dt = 0$

→ Constrained lagrangian (lagrangian multipliers λ_k) :

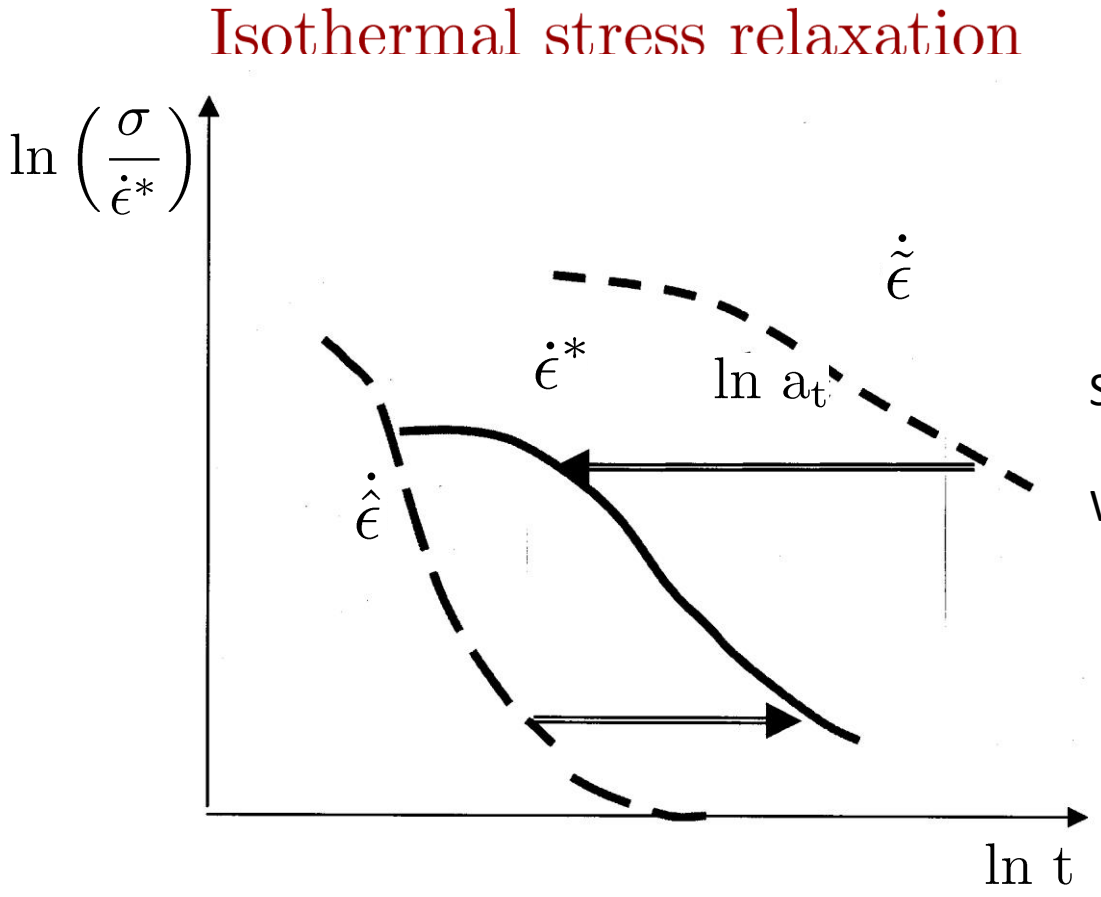
$$L = \frac{\partial \psi}{\partial \boldsymbol{\gamma}} \cdot \dot{\boldsymbol{\gamma}} + \frac{\partial \psi}{\partial \boldsymbol{z}} \cdot \dot{\boldsymbol{z}} + \sum_{k=1}^{N} \lambda_k (\dot{z}_k + \frac{z_k - z_k^r}{\tau_k})$$

Thermodynamic information — Kinetic information

Stationarity condition of $S \Rightarrow$ state laws and kinetic evolution equations for the internal variables

Symmetries and master response for viscous materials

Time temperature superposition for a viscous behaviour



Shift depends on T

Will be determined later on

Master curve at strain rate $\underline{\underline{\dot{\epsilon}}}^*$ obtained by shifting (shifts a_t)

Variational symmetry condition

Invariance of the functional under a group of symmetry :

$$\int_{t_0}^{t_1} L(t, \boldsymbol{\gamma}^{(1)}, \boldsymbol{z}^{(1)}, \boldsymbol{\beta}^{(1)}, \boldsymbol{A}^{(1)}) dt = \int_{\bar{t_0}}^{\bar{t_1}} \bar{L}(\bar{t}, \bar{\boldsymbol{\gamma}}^{(1)}, \bar{\boldsymbol{z}}^{(1)}, \bar{\boldsymbol{\beta}}^{(1)}, \bar{\boldsymbol{A}}^{(1)}) d\bar{t}$$

$$\Leftrightarrow \quad pr^{(1)}\boldsymbol{v} L + L Div \boldsymbol{\xi} = 0 \quad (*)$$

First prolongation :

$$pr^{(1)}\boldsymbol{v} = \boldsymbol{v} + {\boldsymbol{\phi}_{\boldsymbol{\gamma}}}^{t} \frac{\partial}{\partial \dot{\boldsymbol{\gamma}}} + {\boldsymbol{\phi}_{\boldsymbol{z}}}^{t} \frac{\partial}{\partial \dot{\boldsymbol{z}}} + {\boldsymbol{\phi}_{\boldsymbol{\beta}}}^{t} \frac{\partial}{\partial \dot{\boldsymbol{\beta}}} + {\boldsymbol{\phi}_{\boldsymbol{A}}}^{t} \frac{\partial}{\partial \dot{\boldsymbol{A}}}$$

$${\boldsymbol{\phi}_{\boldsymbol{\gamma}}}^{t} = \frac{d}{dt}(\boldsymbol{\phi}_{\boldsymbol{\gamma}} - \boldsymbol{\xi} \cdot \boldsymbol{\gamma}) + \boldsymbol{\xi} \cdot \dot{\boldsymbol{\gamma}}$$

Find all $\boldsymbol{v}$ satisfying (*) with $\quad L = \boldsymbol{\beta} \cdot \dot{\boldsymbol{\gamma}} - \boldsymbol{A} \cdot \dot{\boldsymbol{z}} + \sum_{k=1}^{N} \lambda_k (\dot{z}_k + \frac{z_k - z_k^r}{\tau_k})$

Variational symmetry condition

Profound difference in the status of variables in TIP versus Lie groups:

In TIP, time t is a parameter, control variables $(\varepsilon, \mathrm{T}, \mathrm{z_k})$, observable variables $(\sigma, \mathrm{S}, \mathrm{A_k})$

$$\text{Vector generator } \mathbf{v} = \mathbf{v}_{\text{con}} + \mathbf{v}_{\text{obs}} = \left(\xi \frac{\partial}{\partial \mathrm{t}} + \phi^{\epsilon} \frac{\partial}{\partial \epsilon} + \phi^{\mathrm{T}} \frac{\partial}{\partial \mathrm{T}} + \phi^{\mathrm{z_k}} \frac{\partial}{\partial \mathrm{z_k}}\right) + \left(\phi^{\sigma} \frac{\partial}{\partial \sigma} + \phi^{s} \frac{\partial}{\partial s} + \phi^{A_k} \frac{\partial}{\partial A_k}\right)$$

Components of the observable vector field $\mathbf{v}_{\text{obs}}$ calculated from those of the controllable field $\mathbf{v}_{\text{con}}$:

$$\text{Use state laws : } \begin{cases} \sigma = f_{,\epsilon}(\epsilon, T, z) \\ s = -f_{,T}(\epsilon, T, z) \\ A_i = -f_{,z_i}(\epsilon, T, z) \end{cases} \longrightarrow \begin{cases} \delta\sigma = f_{,\epsilon\epsilon}\delta\epsilon + f_{,T\epsilon}\delta T + f_{,z_k\epsilon}\delta z_k \\ \delta s = -f_{,\epsilon T}\delta\epsilon - f_{,TT}\delta T + f_{,z_k T}\delta z_k \\ \delta A_i = -f_{,\epsilon z_i}\delta\epsilon - f_{,T z_i}\delta T + f_{,z_k z_i}\delta z_k \end{cases}$$

$$\begin{cases} \phi^{\sigma} = f_{,\epsilon\epsilon}\phi^{\epsilon} + f_{,T\epsilon}\phi^{T} + f_{,z_k\epsilon}\phi^{z_k} \\ \phi^{s} = -f_{,\epsilon T}\phi^{\epsilon} - f_{,TT}\phi^{T} - f_{,z_k T}\phi^{z_k} \\ \phi^{A_i} = -f_{,\epsilon z_i}\phi^{\epsilon} - f_{,T z_i}\phi^{T} - f_{,z_k z_i}\phi^{zk} \end{cases}$$

$\rightarrow$ search for symmetries on a subset of the total jet space

Symmetry condition from the kinetic Lagrangian

Independent variable : time t dependent variables : control variables (ϵ, T, z_k)

Variational invariance of l_{thermo} automatically satisfied :

since the generator includes the state laws

$$pr^{(1)}v\,(L_{thermo}) + L_{therm}Div\xi = 0$$

⟶ search for vector fields $\mathbf{v}$ satisfying invariance condition

$pr^{(1)}v\,(L_{kine}) + L_{kine}Div\xi = 0,$ on optimal path $(L_{kine} = 0)$

Equivalent to local symmetry condition $pr^{(1)}v\,(L_{kine}) = 0$

Application: linear viscous behavior

Control variables
(can be controlled during a test)

Observable variables
(function of control variables)

$$\boldsymbol{\gamma} = \left\{ \begin{array}{ccc} \text{uniaxial strain tensor } \varepsilon & \longleftrightarrow & \text{Cauchy stress } \sigma \\ \text{absolute temperature } T & \longleftrightarrow & \text{entropy } s \end{array} \right\} = \boldsymbol{\beta}$$

Helmholtz free energy : $f(\varepsilon, T, z_k)$

$$L = \sigma\dot{\varepsilon} - s\dot{T} - \underbrace{\sum_{k=1}^{N} A_k \dot{z}_k + \sum_{k=1}^{N} \lambda_k \left(\dot{z}_k + \frac{z_k - z_k^r}{\tau_k} \right)}_{\dot{f}}$$

Experimental conditions (assumptions) :

$$\dot{T} = 0 \qquad \dot{\varepsilon} = constant \qquad \tau_k(T) = \frac{h}{kT} \exp\left(\frac{\Delta H - T\Delta S_k}{RT}\right)$$

activation enthalpy

activation entropy of kth dissipative mode

Time-temperature superposition principle

Particular solution $\boldsymbol{v_0}$ satisfying $pr^{(1)}\boldsymbol{v}_0 L + LDiv\boldsymbol{\xi} = 0$

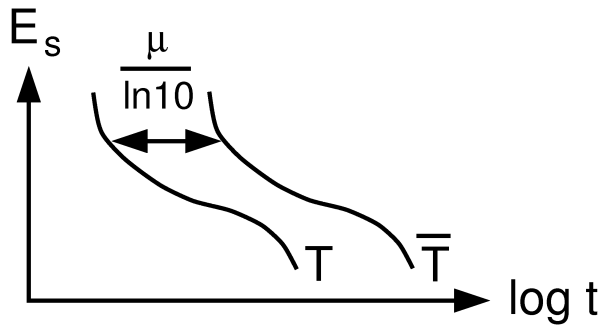
$$\boldsymbol{v}_0 = t\frac{\partial}{\partial t} - \frac{RT^2}{RT + \Delta H}\frac{\partial}{\partial T}$$

$$G_0 \begin{cases} \bar{t} = e^{\mu} t \\ \bar{T} = \exp\left(L_W\left(\frac{\Delta H}{R}\exp\left(\frac{\mu T - T\ln(T^*) + \frac{\Delta H}{R}}{T}\right)\right) - \mu + \ln(T^*) - \frac{\Delta H}{RT}\right) \\ \bar{\sigma} = \sigma \\ \bar{\varepsilon} = \varepsilon \end{cases}$$

→ Invariance property for the secant modulus $E_s(t,T) = \dfrac{\sigma(t,T)}{\varepsilon(t,T)}$

$$E_s(\log t, T) = E_s(\log t + \tfrac{\mu}{\ln 10}, \bar{T})$$

$$\mu(T,\bar{T}) = \frac{\Delta H(T-\bar{T})}{RT\bar{T}} + \ln\frac{T}{\bar{T}}$$



Validation with experimental data

Constitutive equations :

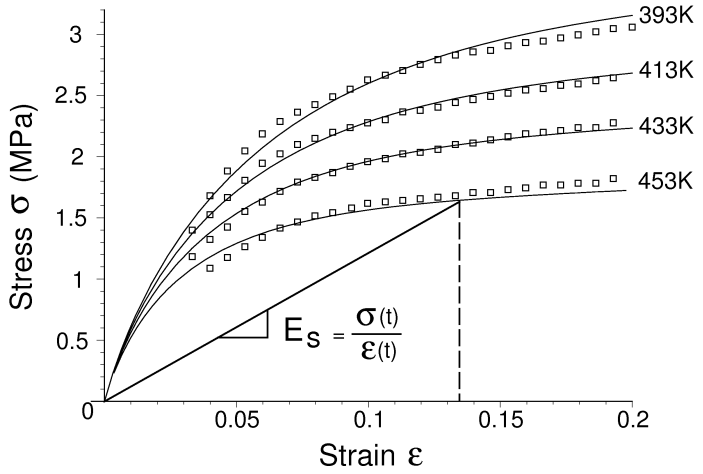
$$\sigma = \sum_{k=1}^{N} \sigma_k$$

$$\dot{\sigma} - E_u\dot{\varepsilon} + \sum_{k=1}^{N} b_k^1 \frac{z_k - c_k\varepsilon}{\tau_k} = 0$$

$$-\dot{s} + \alpha_u E_u\dot{\varepsilon} + \sum_{k=1}^{N} b_k^2 \frac{z_k - c_k\varepsilon}{\tau_k} = 0$$

$$-\dot{A}_i - b_i^1\dot{\varepsilon} + \sum_{k=1}^{N} g_{ik} \frac{z_k - c_k\varepsilon}{\tau_k} = 0$$

$$\dot{\sigma}_k - p_k^0 E_u\dot{\varepsilon} + \frac{\sigma_k - p_k^0 E_r\varepsilon}{\tau_k} = 0$$



□ □ experimental data

—— DNLR curves

$\sigma(t)$ Fit of isothermal tensile curves (PA66)

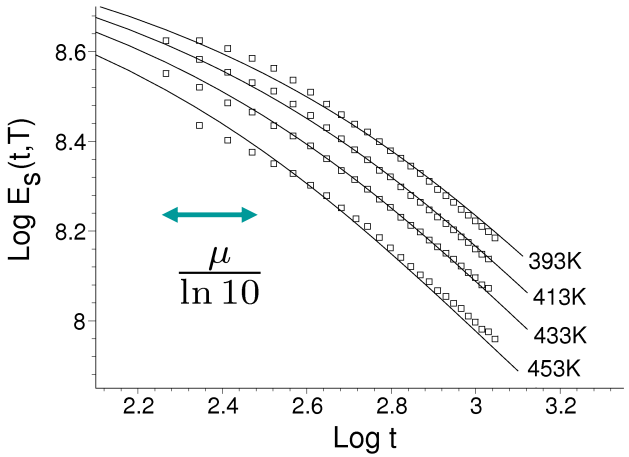
E_u : instantaneous modulus

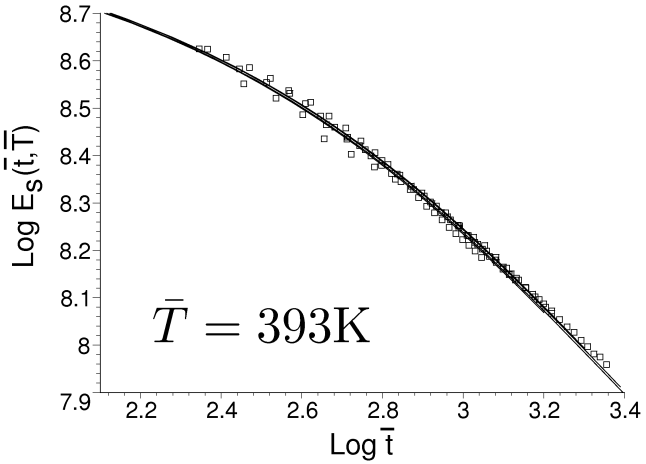
E_r : relaxed modulus

Relaxation spectrum : $\tau_k = \frac{h}{kT}\exp\left(\frac{\Delta H - T\Delta S_k}{RT}\right)$, $p_k^0 = \frac{\sqrt{\tau_k}}{\sum_{i=1}^{N}\sqrt{\tau_i}}$

Construction of master curve

$$E_s(t,T) = \frac{\sigma(t,T)}{\varepsilon(t,T)}$$ module sécant





Groupe de Lie :

$$\bar{t} = e^{\mu} t \quad ; \quad \bar{\sigma} = \sigma \quad ; \quad \bar{\varepsilon} = \varepsilon$$

$$\bar{T} = \exp\left(L_W\left(\frac{\Delta H^+}{R}\exp\left(\frac{\mu T - T\ln(T^*) + \frac{\Delta H^+}{R}}{T}\right)\right) - \mu + \ln(T^*) - \frac{\Delta H^+}{RT}\right)$$

$$\mu(T,\bar{T}) = \frac{\Delta H(T-\bar{T})}{RT\bar{T}} + \ln\frac{T}{\bar{T}} \quad \Rightarrow \quad \Delta H = 12.8 \pm 1.4 \text{ kJ.mol}^{-1}$$

$$\frac{\partial \Delta H}{\partial T} \approx 0 \quad \Rightarrow \quad \text{Validity of the Lie group}$$

$$v_0 = t\frac{\partial}{\partial t} - \frac{RT^2}{RT + \Delta H}\frac{\partial}{\partial T}$$

Néglige variation de volume engendrée par la var. de T, hypothèse faite aussi par WLF

Comparison with the WLF model

Williams, Landel, Ferry empirical formulation for polymers (early seventies)

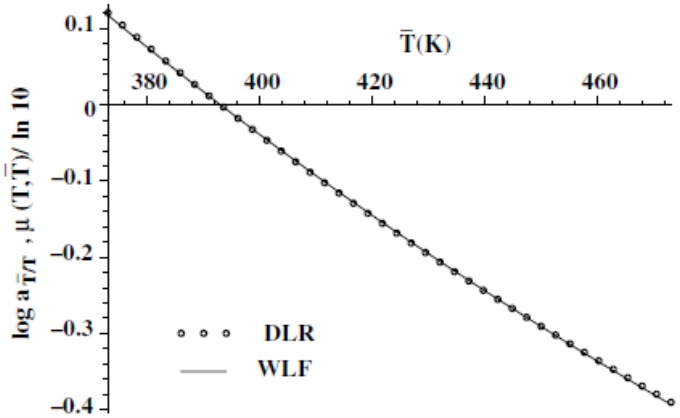
States equivalence property for the secant modulus or relaxation

$$E_s(t,T) = E_s(t a_{T',T}, T') \frac{\rho(T)T}{\rho(T')T'}$$

shift factor given by $\log a_{T',T} = \frac{-C_1(T'-T)}{(C_2+T'-T)}$

Reference temperature = glass transition temperature (here 363°K)

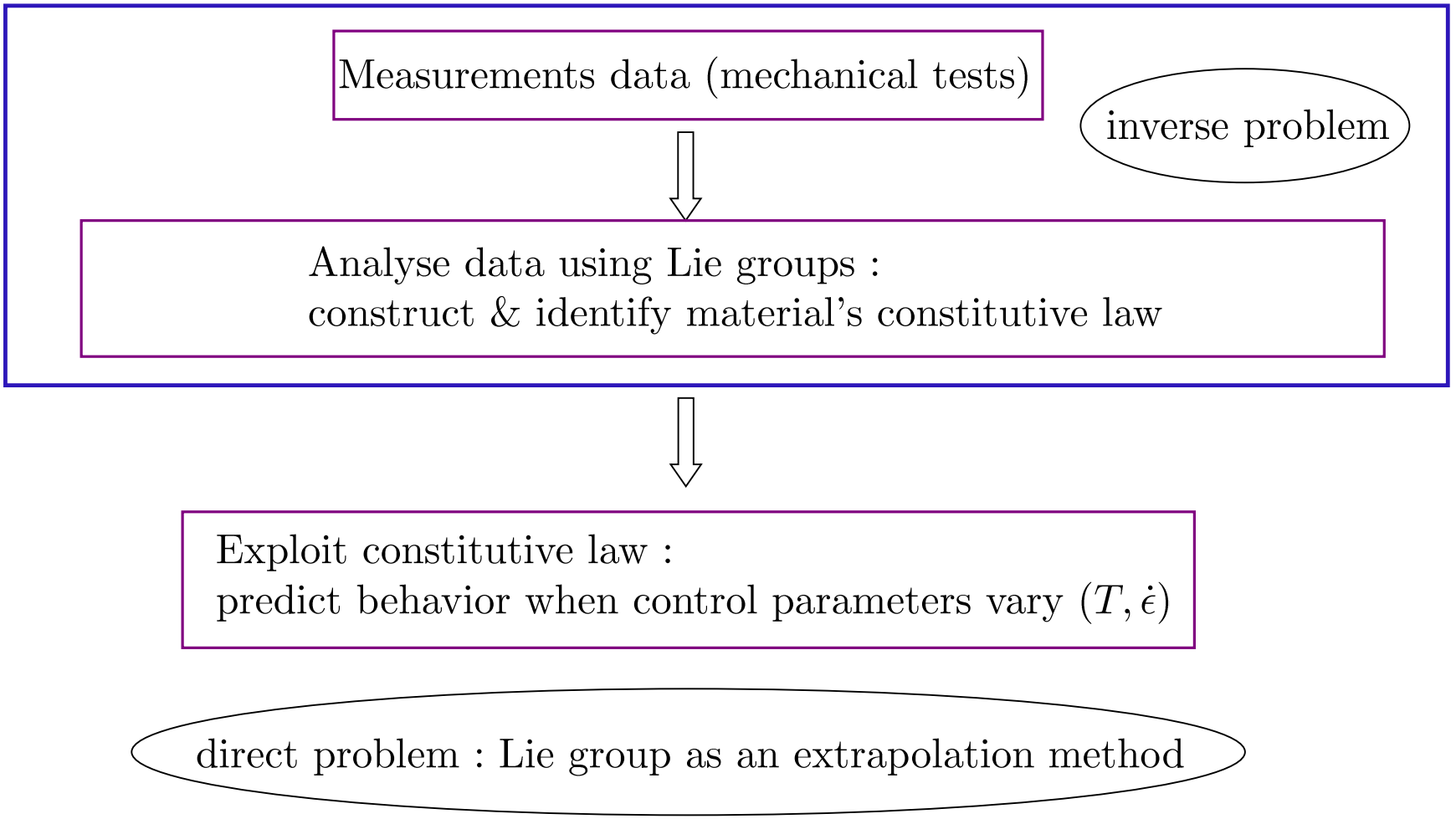
C_1, C_2 material coefficients specific to each polymer



$C_1 = 3, C_2 = 530^\circ K$
'typical values' of WLF coefficients :
$2 \leq C_1 \leq 30 \quad 35K \leq C_2 \leq 220K$ differences due to temperature dependence of mechanical properties

Thus, empirical WLF formula and time–temperature equivalence principle consequence of a particular symmetry of the constitutive equations

Lie symmetries in mechanics of materials : identification of a constitutive law

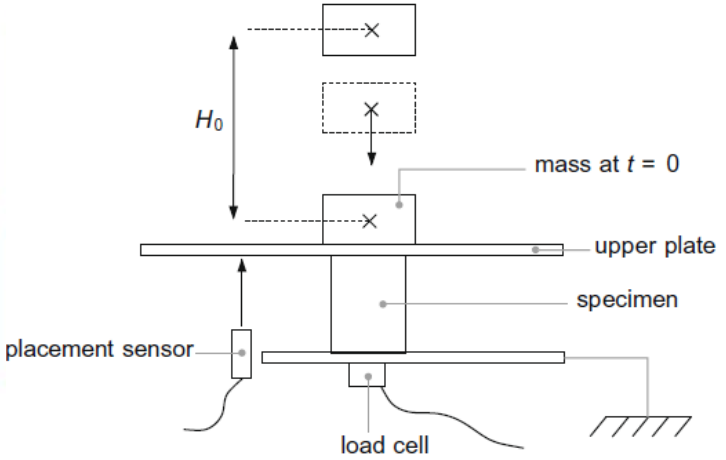


Lie groups construction of material's constitutive law

EU project 'ScreenClean': glue shall be separated from paper fibers during paper recycling

Analyse mechanical response of acrylic stickies under impact

⟶ specimen casted in a cylindrical mould ; stick cooled to remove air bubbles



mass $M = 1kg$ dropped $(V_0 = 0)$ from height H_0

measure displacement $S(t)$ (laser sensor) / compression force $F(t)$ (load sensor)

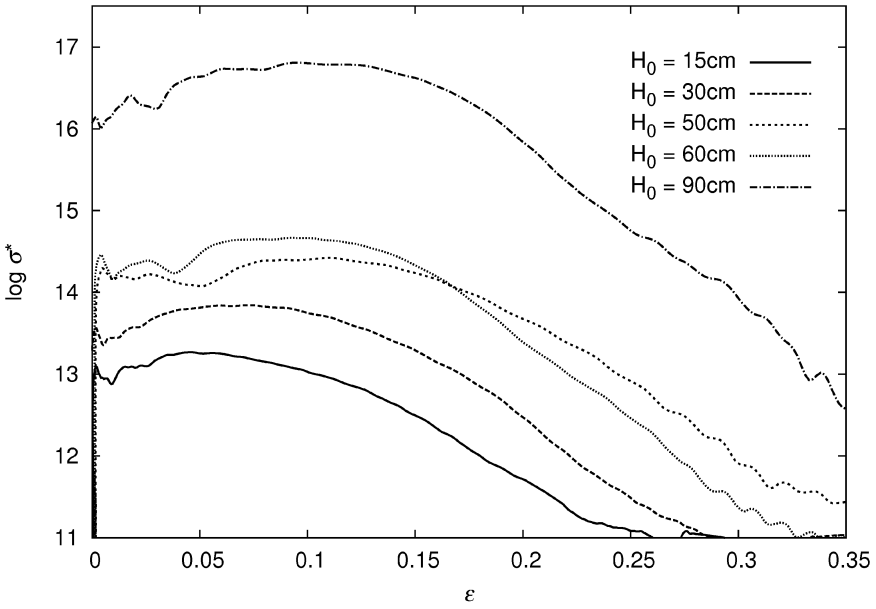
⟶ assume isochoric deformation, thus $S(t) = \frac{S_0 h_0}{h(t)}$, with $h(t) = h_0 - \delta(t)$

⟶ strain rate $\dot{\epsilon} = \frac{\dot{\delta(t)}}{h_0 - \delta(t)}$

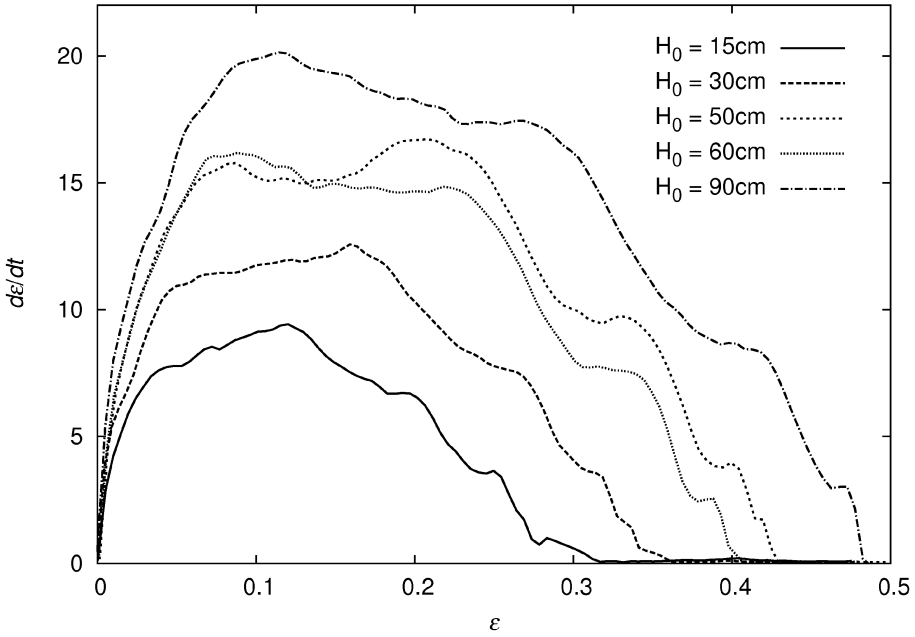
Experimental results

Experiments with 5 heights :
$H_0 = 15cm, H_0 = 30cm, H_0 = 50cm, H_0 = 60cm, H_0 = 90cm$

$\longrightarrow$ associated initial strain rates : $\dot{\epsilon}(0) = \frac{\sqrt{2gH_0}}{h_0}$



stress vs. strain



strain rate vs. strain

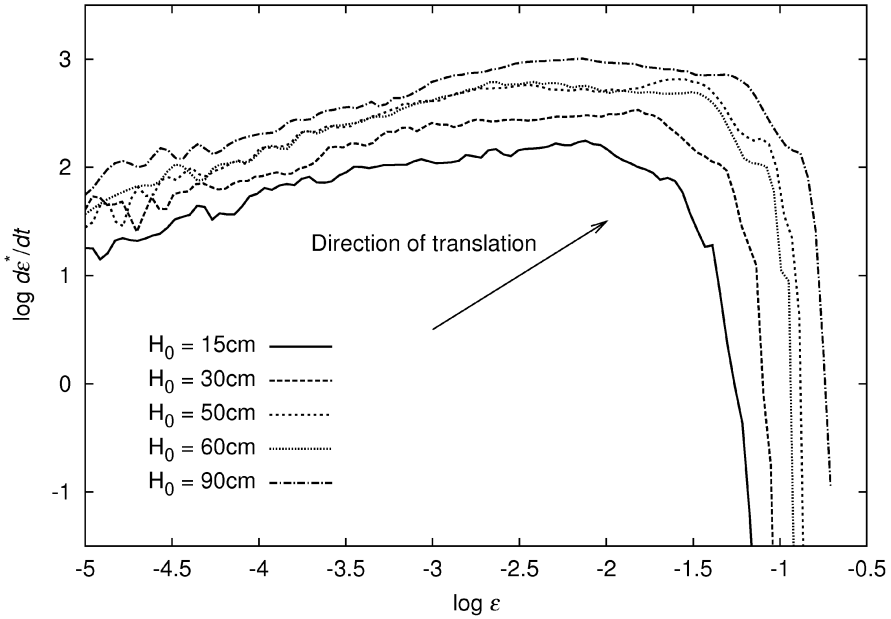
Noise filtering has been done

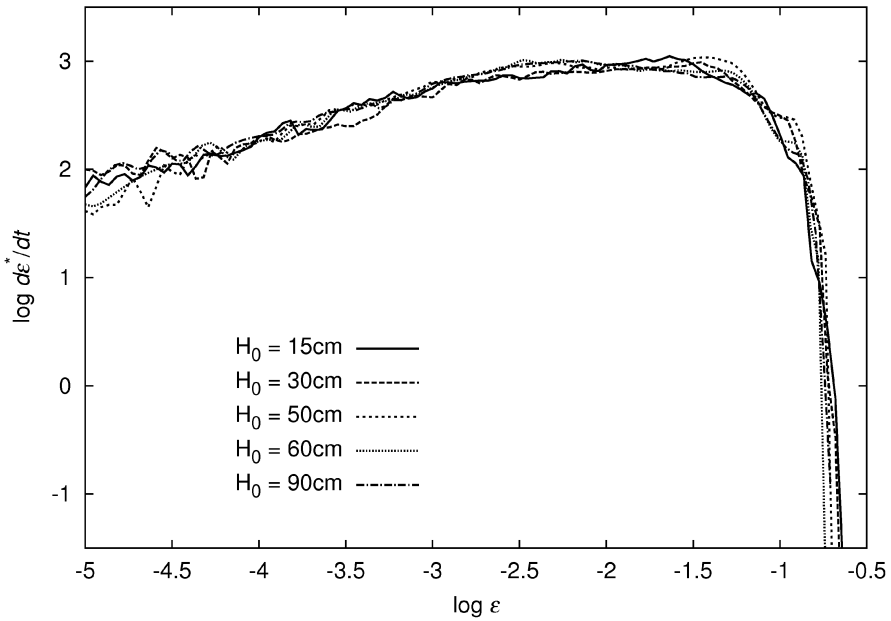
Superposition of measurements : master curve

Superposition of data in $(\epsilon, \dot{\epsilon})$ plane :

$$\log \varepsilon_{90} = \log a_{x\to 90} + \log \varepsilon_x$$
$$\log \dot{\varepsilon}_{90} = \log a_{x\to 90} + \log \dot{\varepsilon}_x$$

Parameter	$\log a_{15\to 90}$	$\log a_{30\to 90}$	$\log a_{50\to 90}$	$\log a_{60\to 90}$	$\log a_{90\to 90}$
Value	0.52	0.36	0.36	0.22	0



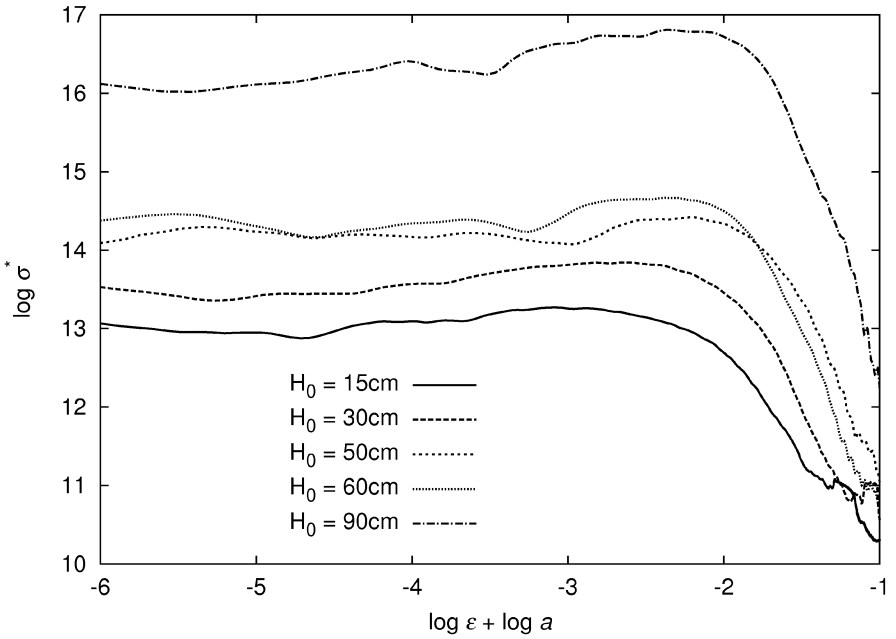


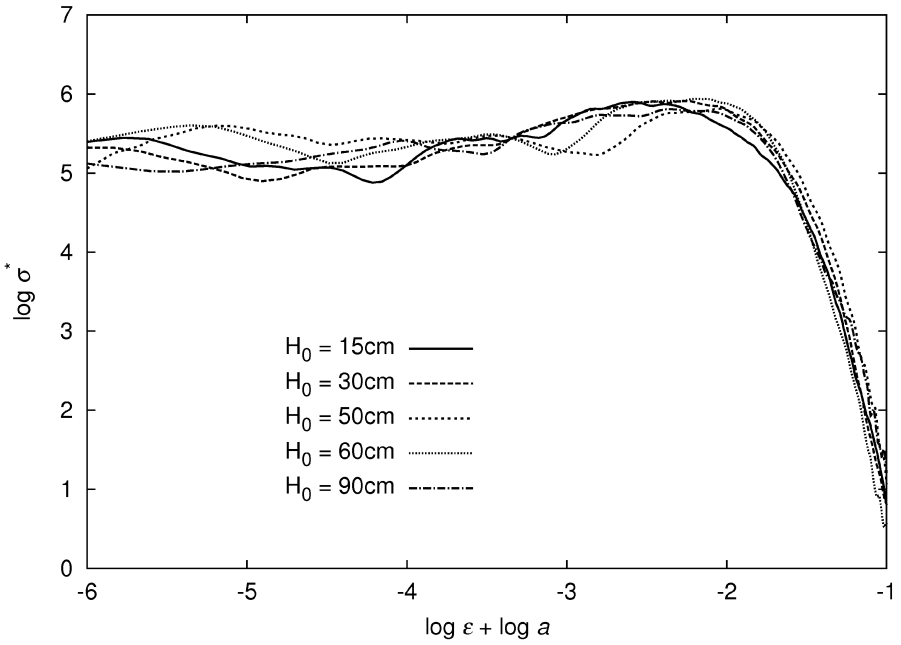
Height of 90cm selected as reference response for the master curve

Superposition of measurements : master curve (2)

Superposition of data in (σ, ϵ) plane : $\log\left(\frac{\sigma^*_{90}}{\sigma^*_0}\right) = b_{x\to 90}\log\left(\frac{\sigma^*_x}{\sigma^*_0}\right)$

Parameter	$b_{15\to 90}$	$b_{30\to 90}$	$b_{50\to 90}$	$b_{60\to 90}$	$b_{90\to 90}$	σ^*_0
Value	2.48	1.97	1.53	1.53	1	59900





Height 90cm: reference response

One parameter Lie group

$b_{x\to 90} = \beta e^{\alpha \log a_{x\to 90}}$ with $\beta = 1.045$, $\alpha = 1.687$ $(R^2 = 99.24)$

Lie group for stickies:

$$\left|\begin{array}{lcll} \varepsilon_{90} & = & e^{\mu_x}\varepsilon_x & \mu_x = \ln a_{x\to 90} \quad (1) \\ \dot{\varepsilon}^*_{90} & = & e^{\mu_x}\dot{\varepsilon}^*_x & (2) \\ \dfrac{\sigma^*_{90}}{\sigma^*_0} & = & \left(\dfrac{\sigma^*_x}{\sigma^*_0}\right)^{\beta e^{\alpha\mu_x}} & (3) \end{array}\right.$$

Viscoplastic constitutive law for acrylic (dynamical loading)
(Naik and Perla, 2008) : $\sigma^* = k_1(\dot{\varepsilon}^*)\varepsilon^{k_2(\dot{\varepsilon}^*)}$

$\varepsilon, \dot{\varepsilon}^*$ independent variables ; accounting for (1),(2),(3) gives symmetry generator

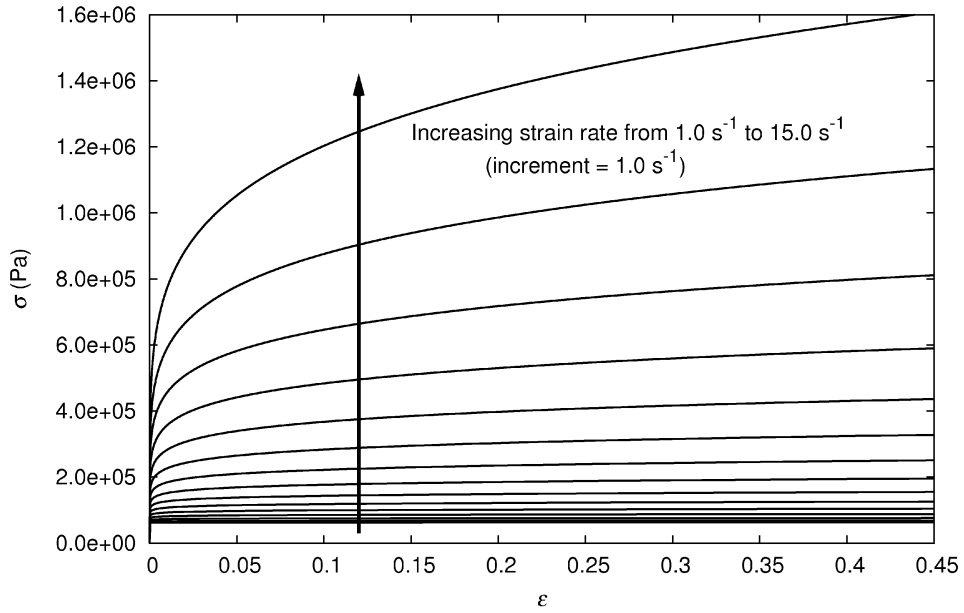
$$\boldsymbol{v} = \varepsilon\frac{\partial}{\partial\varepsilon} + \dot{\varepsilon}^*\frac{\partial}{\partial\dot{\varepsilon}^*} + \alpha\sigma^*\log\left(\frac{\sigma^*}{\sigma^*_0}\right)\frac{\partial}{\partial\sigma^*}$$

Symmetry condition gives $\sigma = \sigma_0\left(c_1\left(\frac{\varepsilon}{\dot{\varepsilon}^*}\right)^{c_2}\right)^{(\dot{\varepsilon}^*)^\alpha}$, with $\sigma_0 = \sigma^*_0 \times 1\text{Pa}$
material parameters obtained by least square adjustment with data :
$c_1 = 1.05 \quad , \quad c_2 = 0.053$

One parameter Lie group (2)

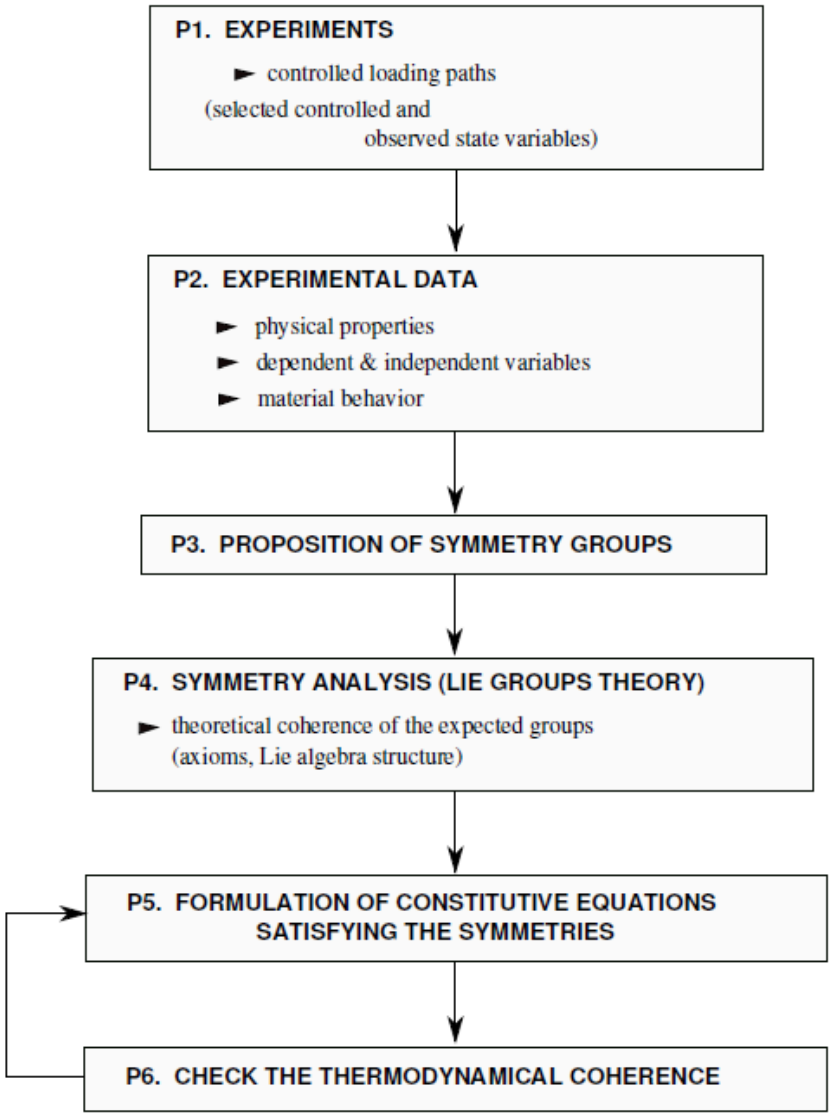
Powerfullness of proposed modelling strategy :
account for a limited set of experimental data in a synthetic manner (Lie group structure)

prediction of material's reponse under various conditions

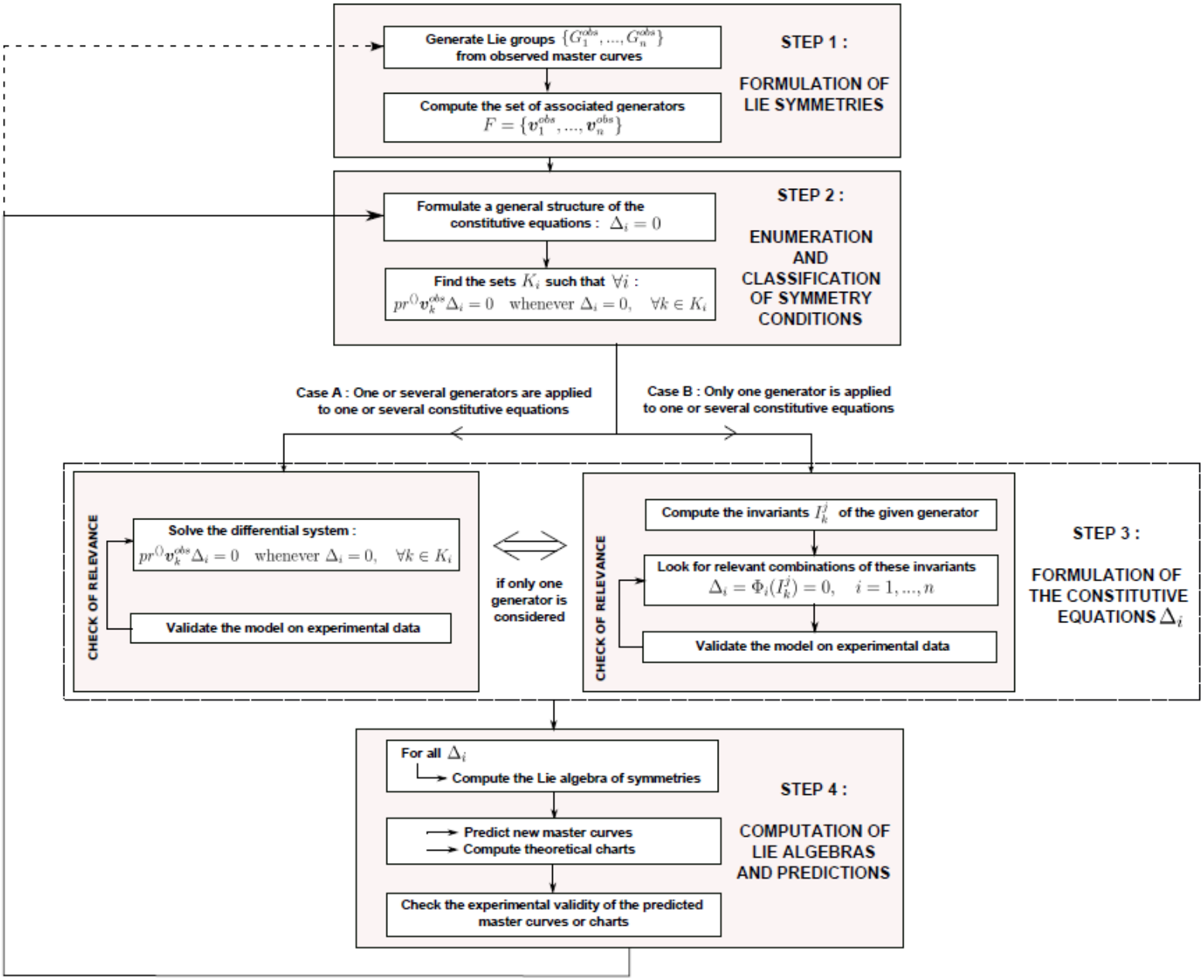


Typical response of viscous polymers

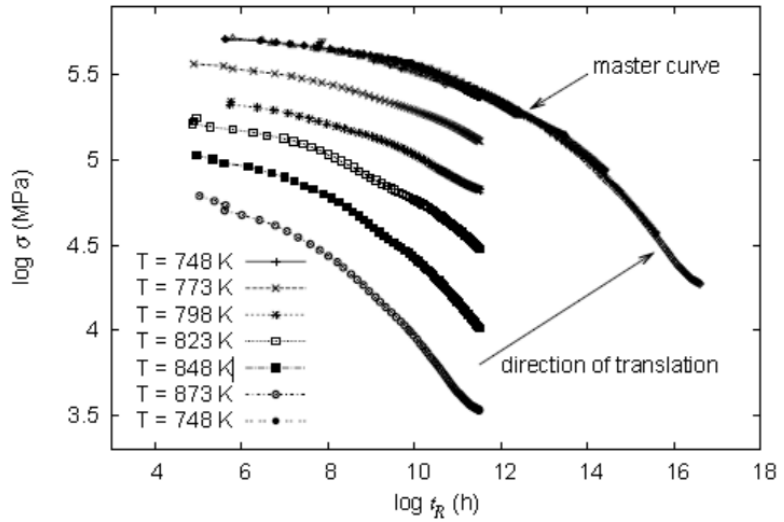
Lie groups method to build constitutive laws: general strategy



Lie groups method to build constitutive laws: general strategy



Creep and rupture of ferritic martensitic steels (9Cr1Mo)



Experimental master curve for rupture

Step 1: construct master responses for creep and rupture

T (K)	748	773	798	823	848	873
μ	0	-25	-50	-75	-100	-125
$a_1(\mu)$	0	0.9	2.0	2.9	4.1	5.1
$b_1(\mu)$	0	0.15	0.32	0.45	0.55	0.74

Table. Values of the shifts $a_1(\mu)$ and $b_1(\mu)$ to superpose a given curve at T on the reference response at $\bar{T} = 748$ K, μ being defined by $\bar{T} = T + \mu$.

$$\begin{cases} \bar{T} &= T + \mu \\ \log \bar{t}_R &= a_1(\mu) + \log t_R \\ \log \bar{\sigma} &= b_1(\mu) + \log \sigma \end{cases}$$

Observable variables: strain rate, time to rupture.
Control variables: applied stress, temperature.

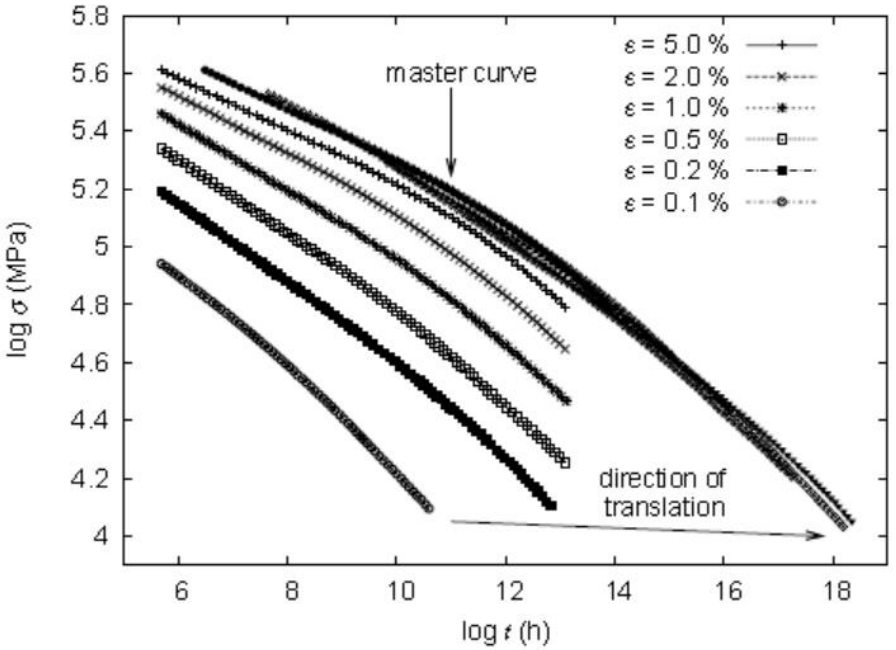
Observed Lie group: $$G_1^{obs} : \begin{cases} \bar{T} &= T + \mu \\ \bar{t}_R &= e^{\alpha\mu} t_R \\ \bar{\sigma} &= e^{\beta\mu} \sigma \end{cases}$$

$\longrightarrow$ group generator:

$$\boldsymbol{v}_1^{obs} = \alpha\, t_R \frac{\partial}{\partial t_R} + \beta\, \sigma \frac{\partial}{\partial \sigma} + \frac{\partial}{\partial T}.$$

$$\alpha = -0.0403636, \quad \beta = -0.00584727$$

Conservation laws for the creep of ferritic martensitic steels



Master curve obtained at the reference strain $\bar{\varepsilon} = 5.0\%$ by shifting the different responses along the $\log t$ and $\log \sigma$ axis.

$\varepsilon(\%)$	5.0	2.0	1.0	0.5	0.2	0.1
μ	0	0.92	1.61	2.30	3.22	3.91
$a_2(\mu)$	0	1.15	2.18	3.33	4.71	6.78
$b_2(\mu)$	0	-0.023	-0.032	-0.046	-0.053	-0.062

Table Values of the shifts $a_2(\mu)$ and $b_2(\mu)$ to superpose a given curve at ε on the reference response at $\bar{\varepsilon} = 5\%$, μ being defined by $\bar{\varepsilon} = e^{\mu}\varepsilon$.

Previous symmetry group for rupture still holds:

$$\boldsymbol{v}_1^{obs} = \alpha\, t_R \frac{\partial}{\partial t_R} + \beta\, \sigma \frac{\partial}{\partial \sigma} + \frac{\partial}{\partial T}.$$

Observed Lie group:

$$G_2^{obs} : \begin{cases} \bar{\varepsilon} &= e^{\mu}\varepsilon \\ \bar{t} &= e^{\gamma\mu} t \\ \bar{\sigma} &= e^{\delta\mu}\sigma \end{cases}.$$

$$\gamma = 1.57167, \quad \delta = -0.0172415.$$

⟶ Group generator:

$$\boldsymbol{v}_2^{obs} = \gamma\, t \frac{\partial}{\partial t} + \delta\sigma \frac{\partial}{\partial \sigma} + \varepsilon \frac{\partial}{\partial \varepsilon}.$$

Two strategies for the construction of the constitutive law

Step 2: Express constitutive law formally as

$$\begin{aligned}\Delta_1 &= t_R - f(\sigma, T) = 0\\ \Delta_2 &= \dot{\varepsilon} - h(t, \sigma, \varepsilon, T) = 0.\end{aligned}$$

f, h unknown functions

apply the symmetry condition $\boldsymbol{v}_1^{obs}$ to Δ_1 and $\boldsymbol{v}_2^{obs}$ to Δ_2.

$$\begin{aligned}pr^{(1)}\boldsymbol{v}_1^{obs}\Delta_1 &= 0, \quad \text{whenever } \Delta_1 = 0 \qquad pr^{(1)}\boldsymbol{v}_1^{obs} = \alpha t_R\frac{\partial}{\partial t_R} + \beta\sigma\frac{\partial}{\partial\sigma} + \frac{\partial}{\partial T}\\ pr^{(1)}\boldsymbol{v}_2^{obs}\Delta_2 &= 0, \quad \text{whenever } \Delta_2 = 0 \qquad pr^{(1)}\boldsymbol{v}_2^{obs} = \gamma t\frac{\partial}{\partial t} + \delta\sigma\frac{\partial}{\partial\sigma} + \varepsilon\frac{\partial}{\partial\varepsilon} + \dot{\varepsilon}(1-\gamma)\frac{\partial}{\partial\dot{\varepsilon}}.\end{aligned}$$

Symmetry generator has been built so far by considering experimental response data and assuming a Lie group structure.

Two possible strategies:

1. Solve previous system with respect to Δ.

2. Find the invariants associated to symmetry generators.
Express constitutive law in terms of suitable combination of invariants.
advantage of identifying constitutive law without solving differential equations

Step 3: Construction of the constitutive law using invariants

Let

$$\boldsymbol{v}^{obs} = \sum_{k=1}^{m} \phi^{p_k} \frac{\partial}{\partial p_k} + \sum_{k=1}^{n} \phi^{u_k} \frac{\partial}{\partial u_k}$$

Observable variables u_k
Parameters p_k

$$\phi^{p_k} = \left.\frac{\partial \Phi^{p_k}}{\partial \mu}\right|_{\mu=0}, \quad \phi^{u_k} = \left.\frac{\partial \Phi^{u_k}}{\partial \mu}\right|_{\mu=0}.$$

If $\boldsymbol{v}^{obs}$ has s non vanishing components amongst $\boldsymbol{\phi}^{p}$ and $\boldsymbol{\phi}^{u}$, it then has $s-1$ invariants $I_1, I_2, \cdots, I_{s-1}$ given by the solution of the characteristic system:

$$\frac{\mathrm{d}p_j}{\phi^{p_j}} = \frac{\mathrm{d}u_i}{\phi^{u_i}}.$$

It is straightforward to show that any function $f(I_1, I_2, \cdots, I_{s-1})$ of the invariants is also invariant under $\boldsymbol{v}^{obs}$

$$\boldsymbol{v}^{obs}[f(I_1, .., I_{s-1})] = \sum_{k=1}^{m} \phi^{p_k} \frac{\partial f}{\partial p_k} + \sum_{k=1}^{n} \phi^{u_k} \frac{\partial f}{\partial u_k} =$$

$$\sum_{k=1}^{m} \phi^{p_k} \sum_{l=1}^{s-1} \frac{\partial f}{\partial I_l} \frac{\partial I_l}{\partial p_k} + \sum_{k=1}^{n} \phi^{u_k} \sum_{l=1}^{s-1} \frac{\partial f}{\partial I_l} \frac{\partial I_l}{\partial u_k} =$$

$$\sum_{l=1}^{s-1} \frac{\partial f}{\partial I_l} \underbrace{\left[\sum_{k=1}^{m} \phi^{p_k} \frac{\partial I_l}{\partial p_k} + \sum_{k=1}^{n} \phi^{u_k} \frac{\partial I_l}{\partial u_k} \right]}_{\boldsymbol{v}^{obs}(I_l)=0} = 0$$

Step 3: Construction of the constitutive law using invariants

Search for functions Σ_1, Σ_2 of invariants I_1, I_2, I_3, such that:

$$\Sigma_1(I_1, I_2) = 0 \quad \Leftrightarrow \quad \Delta_1 = 0$$
$$\Sigma_2(J_1, J_2, J_3) = 0 \quad \Leftrightarrow \quad \Delta_2 = 0$$

I_1, I_2 the invariants of $\boldsymbol{v}_1^{obs}$ given by the solution of the system

$$\frac{\mathrm{d}t_R}{\alpha t_R} = \frac{\mathrm{d}\sigma}{\beta\sigma} = \frac{\mathrm{d}T}{T}$$

J_1, J_2, J_3 the invariants of $\boldsymbol{v}_2^{obs}$ given by the solution of the same characteristic system:

$$\frac{\mathrm{d}t}{\gamma t} = \frac{\mathrm{d}\sigma}{\delta\sigma} = \frac{\mathrm{d}\varepsilon}{\varepsilon} = \frac{\mathrm{d}\dot{\varepsilon}}{(1-\gamma)\dot{\varepsilon}}.$$

$$I_1 = \log t_R - \alpha T, \quad I_2 = \log\sigma - \beta T$$

$$J_1 = \log t - \gamma \log\varepsilon, \quad J_2 = \log\sigma - \delta\log\varepsilon, \quad J_3 = \log\dot{\varepsilon} - (1-\gamma)\log\varepsilon.$$

Step 3: Construction of the rupture law using invariants (2)

Considering rupture, we suggest a relation having the form:

$$\log t_R = \frac{F_1(\sigma)}{T} + F_2(\sigma).$$

Leads to the functional relation between invariants

$$\Sigma_1(I_1, I_2) = \frac{K_1}{I_2} + K_2 I_1 + K_3 I_2 = 0$$

⟶ Expression of rupture time versus temperature & stress:

$$\log t_R = \frac{a}{\log \sigma - \beta T} + b \log \sigma + (\alpha - b\beta)T$$

with $a = -K_1/K_2$ and $b = -K_3/K_2$ new constants.

Good agreement with experimental data.

Linear term in T when combining I_1& I_2: slight difference with Larson-Miller relations.

Step 3: Construction of the creep law using invariants (3)

$$\Sigma_2(J_1, J_2, J_3) = e^{J_3} - Ae^{cJ_1} e^{dJ_2} = \dot{\varepsilon}\varepsilon^{-(1-\gamma)} - At^c\varepsilon^{-c\gamma}\sigma^d\varepsilon^{-d\delta} = 0$$

Leads to strain versus time, stress and temperature:

$$\varepsilon(t) = (1+c)^{-1/\nu}\left[(1+c)\varepsilon_0(\sigma,T)^\nu + A\nu t^{c+1}\sigma^d\right]^{1/\nu}.$$

$$\varepsilon_0(\sigma,T) = \frac{\sigma}{E(T)}$$

Hence the isostrain responses:

$$t(\sigma) = \left[\frac{(c+1)(\varepsilon^\nu - \sigma^\nu E(T)^{-\nu})}{A\nu\sigma^d}\right]^{1/(1+c)}.$$

Coefficients E(T), a,c,d are adjusted.

Step 4: Lie analysis of the creep constitutive laws

Recall creep and rupture constitutive laws of 9Cr1Mo stainless steel:

$$\begin{aligned} \dot{\varepsilon} &= A t^{c} \sigma^{d} \varepsilon^{1-\gamma-c\gamma-d\delta} \quad \text{if } t \le t_R \\ t_R &= \sigma^{b} e^{\frac{\alpha}{\log\sigma-\beta T}+(\alpha-b\beta)T}. \end{aligned}$$

Lie algebra of the creep model:

$$\begin{aligned} pr^{(1)}\boldsymbol{v}_2^1 &= \sigma^d t^{-c}\frac{\partial}{\partial t} + c\dot{\varepsilon}\sigma^d t^{-c-1}\frac{\partial}{\partial \dot{\varepsilon}} \\ pr^{(1)}\boldsymbol{v}_2^2 &= \sigma^d \varepsilon^{1-\nu}\frac{\partial}{\partial \varepsilon} + (1-\nu)\sigma^d \varepsilon^{-\nu}\dot{\varepsilon}\frac{\partial}{\partial \dot{\varepsilon}} \\ pr^{(1)}\boldsymbol{v}_2^3 &= t\frac{\partial}{\partial t} + \left(\frac{c+1}{\nu}\right)\varepsilon\frac{\partial}{\partial \varepsilon} + \left(\frac{c+1-\nu}{\nu}\right)\dot{\varepsilon}\frac{\partial}{\partial \dot{\varepsilon}} \\ pr^{(1)}\boldsymbol{v}_2^4 &= t\frac{\partial}{\partial t} - \left(\frac{c+1}{d}\right)\sigma\frac{\partial}{\partial \sigma} - \dot{\varepsilon}\frac{\partial}{\partial \dot{\varepsilon}} \end{aligned}$$

	$\boldsymbol{v}_2^1$	$\boldsymbol{v}_2^2$	$\boldsymbol{v}_2^3$	$\boldsymbol{v}_2^4$
$\boldsymbol{v}_2^1$	0	0	$(c+1)\boldsymbol{v}_2^1$	$2(c+1)\boldsymbol{v}_2^1$
$\boldsymbol{v}_2^2$	0	0	$(c+1)\boldsymbol{v}_2^2$	$(c+1)\boldsymbol{v}_2^2$
$\boldsymbol{v}_2^3$	$-(c+1)\boldsymbol{v}_2^1$	$-(c+1)\boldsymbol{v}_2^2$	0	0
$\boldsymbol{v}_2^4$	$-2(c+1)\boldsymbol{v}_2^1$	$-(c+1)\boldsymbol{v}_2^2$	0	0

Commutator table of the Lie algebra

In particular, get a master curve:

$$\begin{cases} \log\bar{t} &= \mu + \log t \\ \log\bar{\sigma} &= -\left(\frac{c+1-\nu}{d}\right)\mu + \log\sigma \\ \log\bar{\varepsilon} &= \mu + \log\varepsilon. \end{cases}$$

Step 4: Lie algebra of the rupture law

Two generators:

$$\boldsymbol{v}_1^1 = t_R\left(\frac{b\,(\log\sigma-\beta T)^2-a}{\log\sigma-\beta T}\right)\frac{\partial}{\partial t_R}+\sigma(\log\sigma-\beta T)\frac{\partial}{\partial\sigma}$$

$$\boldsymbol{v}_1^2 = t_R\left(\frac{(\alpha-b\beta)\,(\log\sigma-\beta T)^2+a\beta}{\log\sigma-\beta T}\right)\frac{\partial}{\partial t_R}+(\log\sigma-\beta T)\frac{\partial}{\partial T}$$

	$\boldsymbol{v}_1^1$	$\boldsymbol{v}_1^2$
$\boldsymbol{v}_1^1$	0	$\beta\boldsymbol{v}_1^1+\boldsymbol{v}_1^2$
$\boldsymbol{v}_1^2$	$-\beta\boldsymbol{v}_1^1-\boldsymbol{v}_1^2$	0

Commutator table of the Lie algebra

In particular, get a master curve:

$$\begin{cases}\log\bar{t} &= \mu+\log t\\ \log\bar{\sigma} &= -\left(\frac{e+1-\nu}{d}\right)\mu+\log\sigma\\ \log\bar{\varepsilon} &= \mu+\log\varepsilon.\end{cases}$$

Authors	Invariant(s)
Larson & Miller	$T(\log t+\log B_2)$
Dorn	$\frac{B_1}{T}-\log t$
Monkman-Grant	$\log t_R+m\log\dot{\varepsilon}_{min}$
Modified Monkman-Grant	$\log\left(\frac{t_R}{\varepsilon_R}\right)+m'\log\dot{\varepsilon}_{min}$

Table Some creep invariants encountered in the literature.

Illustrates the general procedure for constructing iso-observables responses

Summary and perspectives (open questions)

• Lie symmetries powerful tool in mechanics of materials: predictive nature, condense mechanical behavior into invariance relations & master responses, thus provide economy of experiments.

• Clarify fundamental significance of symmetries inherent to thermodynamic potentials for materials having a complex rheological behavior.

• Find symmetries for BVP in integro-differential form (hereditary formulations, e.g. viscoelasticity).

• Find approximate symmetries for materials & systems presenting an uncertainty in their behavior (statistical variability in their material properties, ex. biological tissues)
-> stochastic models, approximate symmetries.

• Numerical schemes preserving symmetries & conservation laws for dissipative systems.