Recent news about modeling water-ice phase transitions

Joint work with E. Rocca and J. Sprekels

Pavel Krejčí

Matematický ústav AV ČR
Žitná 25, Praha 1, Czech Republic

ADMAT 2012
Cortona

Multiphase advanced material experiment

Modeling hypotheses

(A1) We consider a bounded 3D container filled with water based substance subject to freezing, assume small displacements inside, and describe the process in Lagrangean coordinates.

Modeling hypotheses

(A1) We consider a bounded 3D container filled with water based substance subject to freezing, assume small displacements inside, and describe the process in Lagrangean coordinates.
The mass conservation is then equivalent to the condition of constant mass density $\varrho_0 > 0$.

Modeling hypotheses

(A1) We consider a bounded 3D container filled with water based substance subject to freezing, assume small displacements inside, and describe the process in Lagrangean coordinates.
The mass conservation is then equivalent to the condition of constant mass density $\varrho_0 > 0$.

(A2) The substance is compressible, and the speed of sound v_0 may depend on the phase.

Modeling hypotheses

(A1) We consider a bounded 3D container filled with water based substance subject to freezing, assume small displacements inside, and describe the process in Lagrangean coordinates.
The mass conservation is then equivalent to the condition of constant mass density $\varrho_0 > 0$.

(A2) The substance is compressible, and the speed of sound v_0 may depend on the phase.

(A3) The evolution is slow, and we neglect shear viscosity and inertia effects.

Modeling hypotheses

(A1) We consider a bounded 3D container filled with water based substance subject to freezing, assume small displacements inside, and describe the process in Lagrangean coordinates.
The mass conservation is then equivalent to the condition of constant mass density $\varrho_0 > 0$.

(A2) The substance is compressible, and the speed of sound v_0 may depend on the phase.

(A3) The evolution is slow, and we neglect shear viscosity and inertia effects.

(A4) We neglect shear stresses.

Modeling hypotheses

(A1) We consider a bounded 3D container filled with water based substance subject to freezing, assume small displacements inside, and describe the process in Lagrangean coordinates.
The mass conservation is then equivalent to the condition of constant mass density $\varrho_0 > 0$.

(A2) The substance is compressible, and the speed of sound v_0 may depend on the phase.

(A3) The evolution is slow, and we neglect shear viscosity and inertia effects.

(A4) We neglect shear stresses.

(A5) The thermal expansion coefficient β is constant, the heat conductivity $\kappa(\chi)$ and specific heat capacity $c_0(\chi) \cdot c_1(\theta)$ may depend on the absolute temperature $\theta > 0$ and on the phase $\chi \in [0, 1]$, $\chi = 1$ means liquid, $\chi = 0$ means solid.

Modeling hypotheses

(A1) We consider a bounded 3D container filled with water based substance subject to freezing, assume small displacements inside, and describe the process in Lagrangean coordinates.
The mass conservation is then equivalent to the condition of constant mass density $\varrho_0 > 0$.

(A2) The substance is compressible, and the speed of sound v_0 may depend on the phase.

(A3) The evolution is slow, and we neglect shear viscosity and inertia effects.

(A4) We neglect shear stresses.

(A5) The thermal expansion coefficient β is constant, the heat conductivity $\kappa(\chi)$ and specific heat capacity $c_0(\chi) \cdot c_1(\theta)$ may depend on the absolute temperature $\theta > 0$ and on the phase $\chi \in [0, 1]$, $\chi = 1$ means liquid, $\chi = 0$ means solid.

(A6) The specific volume of the solid phase $V(0)$ is larger than the specific volume of the liquid phase $V(1)$.

State variables

θ ... absolute temperature

$\mathbf{u}$ ... displacement vector

ε ... strain tensor, $\varepsilon = \nabla_s \mathbf{u}$

χ ... liquid content, $\chi \in [0, 1]$

State variables

- θ ... absolute temperature
- $\mathbf{u}$ ... displacement vector
- ε ... strain tensor, $\boldsymbol{\varepsilon} = \nabla_s \mathbf{u}$
- χ ... liquid content, $\chi \in [0, 1]$

State functions

- $\boldsymbol{\sigma}$ ... stress tensor
- e ... specific internal energy
- s ... specific entropy
- p ... pressure, $\boldsymbol{\sigma} = -p\,\boldsymbol{\delta}$

State variables

θ … absolute temperature

$\mathbf{u}$ … displacement vector

ε … strain tensor, $\varepsilon = \nabla_s \mathbf{u}$

χ … liquid content, $\chi \in [0,1]$

State functions

$\boldsymbol{\sigma}$ … stress tensor

e … specific internal energy

s … specific entropy

p … pressure, $\boldsymbol{\sigma} = -p\,\boldsymbol{\delta}$

$$\boxed{p = -\nu \boldsymbol{\varepsilon}_t : \boldsymbol{\delta} \; -\lambda(\chi)(\boldsymbol{\varepsilon} : \boldsymbol{\delta} - \alpha(1-\chi)) \; +\beta(\theta - \theta_c)}$$

State variables

- θ ... absolute temperature
- $\mathbf{u}$ ... displacement vector
- ε ... strain tensor, $\varepsilon = \nabla_s \mathbf{u}$
- χ ... liquid content, $\chi \in [0,1]$

State functions

- $\boldsymbol{\sigma}$ ... stress tensor
- e ... specific internal energy
- s ... specific entropy
- p ... pressure, $\boldsymbol{\sigma} = -p\,\boldsymbol{\delta}$

$$\boxed{p = -\nu\varepsilon_t : \boldsymbol{\delta} \;\; -\lambda(\chi)(\varepsilon : \boldsymbol{\delta} - \alpha(1-\chi)) \;\; +\beta(\theta - \theta_c)}$$

ν	bulk viscosity
$\boldsymbol{\delta}$	Kronecker tensor

State variables

- θ ... absolute temperature
- $\mathbf{u}$ ... displacement vector
- ε ... strain tensor, $\varepsilon = \nabla_s \mathbf{u}$
- χ ... liquid content, $\chi \in [0, 1]$

State functions

- $\boldsymbol{\sigma}$ ... stress tensor
- e ... specific internal energy
- s ... specific entropy
- p ... pressure, $\boldsymbol{\sigma} = -p\,\boldsymbol{\delta}$

$$\boxed{p = -\nu \varepsilon_t : \boldsymbol{\delta} \; -\lambda(\chi)(\varepsilon : \boldsymbol{\delta} - \alpha(1-\chi)) \; +\beta(\theta - \theta_c)}$$

ν	bulk viscosity
$\boldsymbol{\delta}$	Kronecker tensor
$\lambda(\chi) = v_0^2(\chi)/V(\chi)$	bulk elasticity modulus
$\alpha = (V(0) - V(1))/V(1)$	phase expansion coefficient

State variables

- θ ... absolute temperature
- $\mathbf{u}$ ... displacement vector
- ε ... strain tensor, $\varepsilon = \nabla_s \mathbf{u}$
- χ ... liquid content, $\chi \in [0, 1]$

State functions

- $\boldsymbol{\sigma}$ ... stress tensor
- e ... specific internal energy
- s ... specific entropy
- p ... pressure, $\boldsymbol{\sigma} = -p\,\boldsymbol{\delta}$

$$p = -\nu\varepsilon_t : \boldsymbol{\delta} \ -\lambda(\chi)(\varepsilon : \boldsymbol{\delta} - \alpha(1-\chi)) \ +\beta(\theta - \theta_c)$$

ν	bulk viscosity
$\boldsymbol{\delta}$	Kronecker tensor
$\lambda(\chi) = v_0^2(\chi)/V(\chi)$	bulk elasticity modulus
$\alpha = (V(0) - V(1))/V(1)$	phase expansion coefficient
β	thermal expansion coefficient
θ_c	freezing point at standard pressure

Specific volume of water	$V(1) = 1/\varrho_0$	10^{-3}	m^3/kg
Specific volume of ice	$V(0)$	$1.09 \cdot 10^{-3}$	m^3/kg
Speed of sound in water	$v_0(1)$	$1.5 \cdot 10^3$	m/s
Speed of sound in ice	$v_0(0)$	$3.12 \cdot 10^3$	m/s
Bulk elasticity modulus of water	$\lambda(1) = v_0(1)^2/V(1)$	$2.25 \cdot 10^9$	$Pa = J/m^3 = kg/m\,s^2$
Bulk elasticity modulus of ice	$\lambda(0) = v_0(0)^2/V(0)$	$9 \cdot 10^9$	$Pa = J/m^3 = kg/m\,s^2$
Bulk viscosity	ν	$8.9 \cdot 10^{-4}$	$Pa/s = kg/m\,s^3$
Specific heat capacity of water	$c_0(1)$	$4.2 \cdot 10^3$	$J/kg\,K = m^2/s^2K$
Specific heat capacity of ice	$c_0(0)$	$2.1 \cdot 10^3$	$J/kg\,K = m^2/s^2K$
Latent heat	L_0	$3.34 \cdot 10^5$	$J/kg = m^2/s^2$
Thermal expansion coefficient	β	$4.5 \cdot 10^5$	$J/m^3K = kg/m\,s^2K$
Freezing point at standard pressure	θ_c	273	K
Standard pressure	p_0	10^5	$Pa = J/m^3 = kg/m\,s^2$
Phase expansion coefficient	$\alpha = (V(0) - V(1))/V(1)$	0.09	
Gravity constant	g	9.8	m/s^2

Table: Physical constants

Balance equations

In a bounded connected $C^{1,1}$ container $\Omega \subset \mathbb{R}^3$ subject to a constant gravity force $\mathbf{g}_{grav}$, we consider for times $t \geq 0$ the system

$$-\mathrm{div}\, \boldsymbol{\sigma} = \mathbf{g}_{grav} \qquad \text{mechanical equilibrium}$$

Balance equations

In a bounded connected $C^{1,1}$ container $\Omega \subset \mathbb{R}^3$ subject to a constant gravity force $\mathbf{g}_{grav}$, we consider for times $t \geq 0$ the system

$$\nabla p = \mathbf{g}_{grav} \qquad \text{mechanical equilibrium}$$

Balance equations

In a bounded connected $C^{1,1}$ container $\Omega \subset \mathbb{R}^3$ subject to a constant gravity force $\mathbf{g}_{grav}$, we consider for times $t \geq 0$ the system

$$\nabla p = \mathbf{g}_{grav} \qquad \text{mechanical equilibrium}$$

$$\varrho_0 e_t + \operatorname{div} \mathbf{q} = \boldsymbol{\sigma} : \varepsilon_t \qquad \text{internal energy balance}$$

where $\mathbf{q}$ is the heat flux.

Balance equations

In a bounded connected $C^{1,1}$ container $\Omega \subset \mathbb{R}^3$ subject to a constant gravity force $\mathbf{g}_{grav}$, we consider for times $t \geq 0$ the system

$$
\begin{aligned}
\nabla p &= \mathbf{g}_{grav} && \text{mechanical equilibrium} \\
\varrho_0 e_t + \operatorname{div} \mathbf{q} &= \boldsymbol{\sigma} : \varepsilon_t && \text{internal energy balance} \\
\varrho_0 s_t + \operatorname{div} \frac{\mathbf{q}}{\theta} &\geq 0 && \text{entropy balance}
\end{aligned}
$$

where $\mathbf{q}$ is the heat flux.

Balance equations

In a bounded connected $C^{1,1}$ container $\Omega \subset \mathbb{R}^3$ subject to a constant gravity force $\mathbf{g}_{grav}$, we consider for times $t \geq 0$ the system

$$\begin{aligned} \nabla p &= \mathbf{g}_{grav} && \text{mechanical equilibrium} \\ \varrho_0 e_t + \operatorname{div} \mathbf{q} &= \boldsymbol{\sigma} : \varepsilon_t && \text{internal energy balance} \\ \varrho_0 s_t + \operatorname{div} \frac{\mathbf{q}}{\theta} &\geq 0 && \text{entropy balance} \end{aligned}$$

where $\mathbf{q}$ is the heat flux.

Specific free energy

$$\begin{aligned} f = e - \theta\, s \;&=\; c_0(\chi) f_1(\theta) + \frac{\lambda(\chi)}{2\varrho_0}\big(\varepsilon : \boldsymbol{\delta} - \alpha(1-\chi)\big)^2 \\ &\quad - \frac{\beta}{\varrho_0}(\theta - \theta_c)\varepsilon : \boldsymbol{\delta} + L_0\left(\chi\left(1 - \frac{\theta}{\theta_c}\right) + I(\chi)\right). \end{aligned}$$

I ... indicator function of the interval $[0, 1]$, L_0 ... latent heat.

Balance equations

In a bounded connected $C^{1,1}$ container $\Omega \subset \mathbb{R}^3$ subject to a constant gravity force $\mathbf{g}_{grav}$, we consider for times $t \geq 0$ the system

$$
\begin{aligned}
\nabla p &= \mathbf{g}_{grav} && \text{mechanical equilibrium} \\
\varrho_0 e_t + \operatorname{div} \mathbf{q} &= \boldsymbol{\sigma} : \varepsilon_t && \text{internal energy balance} \\
\chi_t \cdot \partial_\chi f &\leq 0 && \text{entropy balance}
\end{aligned}
$$

where $\mathbf{q}$ is the heat flux, $\mathbf{q} \cdot \nabla\theta \leq 0$, $\quad s = -\partial_\theta f$.

Specific free energy

$$
\begin{aligned}
f = e - \theta s &= c_0(\chi) f_1(\theta) + \frac{\lambda(\chi)}{2\varrho_0}\big(\varepsilon : \boldsymbol{\delta} - \alpha(1-\chi)\big)^2 \\
&\quad - \frac{\beta}{\varrho_0}(\theta - \theta_c)\varepsilon : \boldsymbol{\delta} + L_0\Big(\chi\Big(1 - \frac{\theta}{\theta_c}\Big) + I(\chi)\Big).
\end{aligned}
$$

I ... indicator function of the interval $[0,1]$, L_0 ... latent heat.

Balance equations

In a bounded connected $C^{1,1}$ container $\Omega \subset \mathbb{R}^3$ subject to a constant gravity force $\mathbf{g}_{grav}$, we consider for times $t \geq 0$ the system

$$
\begin{aligned}
\nabla p &= \mathbf{g}_{grav} && \text{mechanical equilibrium} \\
\varrho_0 e_t + \operatorname{div} \mathbf{q} &= \boldsymbol{\sigma} : \varepsilon_t && \text{internal energy balance} \\
-\gamma_0 \chi_t &\in \partial_\chi f && \text{phase dynamics}
\end{aligned}
$$

where $\mathbf{q}$ is the heat flux, $\mathbf{q} \cdot \nabla\theta \leq 0\,, \quad s = -\partial_\theta f\,.$

Specific free energy

$$
\begin{aligned}
f = e - \theta\, s \;\; &= \;\; c_0(\chi) f_1(\theta) + \frac{\lambda(\chi)}{2\varrho_0}\big(\varepsilon : \boldsymbol{\delta} - \alpha(1-\chi)\big)^2 \\
&\quad - \frac{\beta}{\varrho_0}(\theta - \theta_c)\varepsilon : \boldsymbol{\delta} + L_0\Big(\chi\Big(1 - \frac{\theta}{\theta_c}\Big) + I(\chi)\Big)\,.
\end{aligned}
$$

I ... indicator function of the interval $[0,1]$, L_0 ... latent heat.

Balance equations II

The mechanical balance equation can be written in the form $p(x,t) = P(t) - \varrho_0 g x_3$ with an unknown function $P(t)$ of time only.

Balance equations II

The mechanical balance equation can be written in the form $p(x,t) = P(t) - \varrho_0 g x_3$ with an unknown function $P(t)$ of time only.

Put $U = \boldsymbol{\varepsilon} : \boldsymbol{\delta} = \operatorname{div} \mathbf{u}$, $L = \varrho_0 L_0, c = \varrho_0 c_0, \gamma = \varrho_0 \gamma_0$, and assume the Fourier law $\mathbf{q} = -\kappa(\chi)\nabla\theta$.

Balance equations II

The mechanical balance equation can be written in the form $p(x,t) = P(t) - \varrho_0 g x_3$ with an unknown function $P(t)$ of time only.

Put $U = \varepsilon : \delta = \mathrm{div}\,\mathbf{u}$, $L = \varrho_0 L_0, c = \varrho_0 c_0, \gamma = \varrho_0 \gamma_0$, and assume the Fourier law $\mathbf{q} = -\kappa(\chi)\nabla\theta$.
The full dynamical problem reads

$$
\begin{aligned}
c(\chi) e_1(\theta)_t - \mathrm{div}\,(\kappa(\chi)\nabla\theta) &= c'(\chi)\chi_t(f_1(\theta) - e_1(\theta)) \\
&\quad + \nu U_t^2 - \beta\theta U_t + \gamma\chi_t^2 - L\frac{\theta}{\theta_c}\chi_t\,,
\end{aligned}
$$

Balance equations II

The mechanical balance equation can be written in the form $p(x,t) = P(t) - \varrho_0 g x_3$ with an unknown function $P(t)$ of time only.

Put $U = \varepsilon : \delta = \operatorname{div} \mathbf{u}$, $L = \varrho_0 L_0, c = \varrho_0 c_0, \gamma = \varrho_0 \gamma_0$, and assume the Fourier law $\mathbf{q} = -\kappa(\chi)\nabla\theta$.
The full dynamical problem reads

$$\begin{aligned} c(\chi)e_1(\theta)_t - \operatorname{div}(\kappa(\chi)\nabla\theta) &= c'(\chi)\chi_t(f_1(\theta) - e_1(\theta)) \\ &\quad + \nu U_t^2 - \beta\theta U_t + \gamma\chi_t^2 - L\frac{\theta}{\theta_c}\chi_t\,, \\ \nu U_t + \lambda(\chi)(U - \alpha(1-\chi)) - \beta(\theta - \theta_c) &= \varrho_0 g x_3 - P(t)\,, \end{aligned}$$

Balance equations II

The mechanical balance equation can be written in the form $p(x,t) = P(t) - \varrho_0 g x_3$ with an unknown function $P(t)$ of time only.

Put $U = \boldsymbol{\varepsilon} : \boldsymbol{\delta} = \operatorname{div} \mathbf{u}$, $L = \varrho_0 L_0, c = \varrho_0 c_0, \gamma = \varrho_0 \gamma_0$, and assume the Fourier law $\mathbf{q} = -\kappa(\chi)\nabla\theta$.
The full dynamical problem reads

$$\begin{aligned} c(\chi)e_1(\theta)_t - \operatorname{div}(\kappa(\chi)\nabla\theta) &= c'(\chi)\chi_t(f_1(\theta) - e_1(\theta)) \\ &\quad + \nu U_t^2 - \beta\theta U_t + \gamma\chi_t^2 - L\frac{\theta}{\theta_c}\chi_t\,, \\ \nu U_t + \lambda(\chi)(U - \alpha(1-\chi)) - \beta(\theta - \theta_c) &= \varrho_0 g x_3 - P(t)\,, \\ -\gamma\chi_t - \frac{\lambda'(\chi)}{2}(U - \alpha(1-\chi))^2 &- \alpha\lambda(\chi)(U - \alpha(1-\chi)) \\ &\in c'(\chi)\left(f_1(\theta) - f_1(\theta_c)\right) + L\left(1 - \frac{\theta}{\theta_c}\right) + \partial I(\chi) \end{aligned}$$

The function $P(t)$ is determined from the boundary condition for $\mathbf{u}$.

Elastic boundary

Assume that the normal displacement on the boundary is proportional to the difference between the inner and outer pressure, that is,
$p(x,t) - p_0(t) = k(x)\mathbf{u}\cdot\mathbf{n}$ on $\partial\Omega$.

Elastic boundary

Assume that the normal displacement on the boundary is proportional to the difference between the inner and outer pressure, that is, $p(x,t) - p_0(t) = k(x)\mathbf{u}\cdot\mathbf{n}$ on $\partial\Omega$. Hence,

$$\int_\Omega U(x,t)\,\mathrm{d}x = \int_{\partial\Omega} \mathbf{u}\cdot\mathbf{n}\,\mathrm{d}s(x) = \int_{\partial\Omega} \frac{1}{k(x)}\left(P(t) - \varrho_0 g x_3 - p_0(t)\right)\mathrm{d}s(x).$$

Elastic boundary

Assume that the normal displacement on the boundary is proportional to the difference between the inner and outer pressure, that is, $p(x,t) - p_0(t) = k(x)\mathbf{u}\cdot\mathbf{n}$ on $\partial\Omega$. Hence,

$$\int_\Omega U(x,t)\,\mathrm{d}x = \int_{\partial\Omega} \mathbf{u}\cdot\mathbf{n}\,\mathrm{d}s(x) = \int_{\partial\Omega} \frac{1}{k(x)}(P(t) - \varrho_0 g x_3 - p_0(t))\,\mathrm{d}s(x).$$

We obtain

$$P = K_\Gamma \int_\Omega U\,\mathrm{d}x + \tilde{P},$$

Elastic boundary

Assume that the normal displacement on the boundary is proportional to the difference between the inner and outer pressure, that is, $p(x,t) - p_0(t) = k(x)\mathbf{u}\cdot\mathbf{n}$ on $\partial\Omega$. Hence,

$$\int_\Omega U(x,t)\,\mathrm{d}x = \int_{\partial\Omega} \mathbf{u}\cdot\mathbf{n}\,\mathrm{d}s(x) = \int_{\partial\Omega} \frac{1}{k(x)}(P(t) - \varrho_0 g x_3 - p_0(t))\,\mathrm{d}s(x).$$

We obtain

$$P = K_\Gamma \int_\Omega U\,\mathrm{d}x + \tilde{P}, \ \frac{1}{K_\Gamma} = \int_{\partial\Omega} \frac{\mathrm{d}s(x)}{k(x)},$$

Elastic boundary

Assume that the normal displacement on the boundary is proportional to the difference between the inner and outer pressure, that is, $p(x,t) - p_0(t) = k(x)\mathbf{u}\cdot\mathbf{n}$ on $\partial\Omega$. Hence,

$$\int_\Omega U(x,t)\,\mathrm{d}x = \int_{\partial\Omega} \mathbf{u}\cdot\mathbf{n}\,\mathrm{d}s(x) = \int_{\partial\Omega} \frac{1}{k(x)}(P(t) - \varrho_0 g x_3 - p_0(t))\,\mathrm{d}s(x).$$

We obtain

$$P = K_\Gamma \int_\Omega U\,\mathrm{d}x + \tilde{P},\ \frac{1}{K_\Gamma} = \int_{\partial\Omega} \frac{\mathrm{d}s(x)}{k(x)},\ \tilde{P} = p_0 + K_\Gamma \int_{\partial\Omega} \frac{\varrho_0 g x_3}{k(x)}\,\mathrm{d}s(x),$$

Elastic boundary

Assume that the normal displacement on the boundary is proportional to the difference between the inner and outer pressure, that is, $p(x,t) - p_0(t) = k(x)\mathbf{u}\cdot\mathbf{n}$ on $\partial\Omega$. Hence,

$$\int_\Omega U(x,t)\,\mathrm{d}x = \int_{\partial\Omega} \mathbf{u}\cdot\mathbf{n}\,\mathrm{d}s(x) = \int_{\partial\Omega} \frac{1}{k(x)}(P(t) - \varrho_0 g x_3 - p_0(t))\,\mathrm{d}s(x).$$

We obtain

$$P = K_\Gamma \int_\Omega U\,\mathrm{d}x + \tilde{P}, \ \frac{1}{K_\Gamma} = \int_{\partial\Omega} \frac{\mathrm{d}s(x)}{k(x)}, \ \tilde{P} = p_0 + K_\Gamma \int_{\partial\Omega} \frac{\varrho_0 g x_3}{k(x)}\,\mathrm{d}s(x),$$

and the mechanical equilibrium equation has the form

$$\nu U_t + \lambda(\chi)(U - \alpha(1-\chi)) - \beta(\theta - \theta_c) = \varrho_0 g x_3 - K_\Gamma \int_\Omega U\,\mathrm{d}x - \tilde{P}(t).$$

Elastoplastic boundary I

The response of the boundary to pressure changes is assumed to be elastoplastic according to the Prager hardening model. We assume that the normal displacement $\mathbf{u} \cdot \mathbf{n}$ is decomposed into the sum $\mathbf{u} \cdot \mathbf{n} = u^e + u^p$ of an elastic component u^e and plastic component u^p.

Elastoplastic boundary I

The response of the boundary to pressure changes is assumed to be elastoplastic according to the Prager hardening model. We assume that the normal displacement $\mathbf{u}\cdot\mathbf{n}$ is decomposed into the sum $\mathbf{u}\cdot\mathbf{n} = u^e + u^p$ of an elastic component u^e and plastic component u^p. Let also the pressure difference $P_0(x,t) = P(t) - \varrho_0 g x_3 - p_0(t)$ be decomposed into a sum $P_0(x,t) = p^h(x,t) + p^b(x,t)$ of a kinematic hardening component p^h and a backstress p^b.

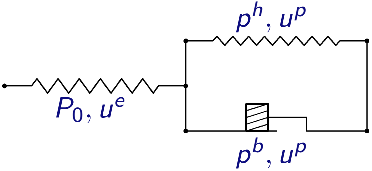
Elastoplastic boundary I

The response of the boundary to pressure changes is assumed to be elastoplastic according to the Prager hardening model. We assume that the normal displacement $\mathbf{u}\cdot\mathbf{n}$ is decomposed into the sum $\mathbf{u}\cdot\mathbf{n} = u^e + u^p$ of an elastic component u^e and plastic component u^p. Let also the pressure difference $P_0(x,t) = P(t) - \varrho_0 g x_3 - p_0(t)$ be decomposed into a sum $P_0(x,t) = p^h(x,t) + p^b(x,t)$ of a kinematic hardening component p^h and a backstress p^b. The boundary condition for $\mathbf{u}$ then reads

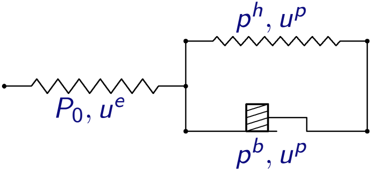
$$
\begin{aligned}
P_0(x,t) &= k(x)u^e(x,t)\,,\\
p^h(x,t) &= b(x)u^p(x,t)\,,\\
|p^b(x,t)| &\le r(x) \ \text{ a.e.}\,,\\
\frac{\partial u^p}{\partial t}(p^b(x,t) - y) &\ge 0 \ \text{ a.e.}\,, \quad \forall y \in [-r(x), r(x)]
\end{aligned}
$$

with given positive measurable functions $k(x)$ (elasticity of the boundary), $b(x)$ (hardening coefficient), and $r(x)$ (yield stress).

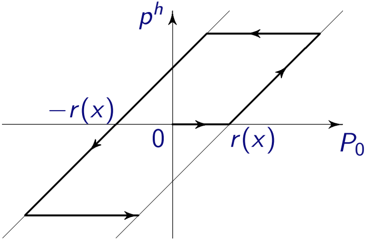
An analogical model



An analogical model



The phase diagram



Elastoplastic boundary II

The variational inequality

$$\frac{\partial p^h(x,t)}{\partial t}(P_0(x,t) - p^h(x,t) - y) \ \geq \ 0 \ \text{ a.e.} \quad \forall y \in [-r(x), r(x)]\,,$$

with initial condition

$$p^h(x,0) \ = \ \min\{P_0(x,0) + r(x), \max\{0, P_0(x,0) - r(x)\}\}$$

corresponding to the initially undeformed state, defines the so-called play operator

$$p^h(x,t) \ = \ \mathfrak{p}_{r(x)}[P_0](x,t)$$

with threshold $r(x)$.

Elastoplastic boundary II

The variational inequality

$$\frac{\partial p^h(x,t)}{\partial t}(P_0(x,t) - p^h(x,t) - y) \;\geq\; 0 \;\; \text{a.e.} \quad \forall y \in [-r(x), r(x)]\,,$$

with initial condition

$$p^h(x,0) \;=\; \min\{P_0(x,0) + r(x), \max\{0, P_0(x,0) - r(x)\}\}$$

corresponding to the initially undeformed state, defines the so-called play operator

$$p^h(x,t) \;=\; \mathfrak{p}_{r(x)}[P_0](x,t)$$

with threshold $r(x)$.

Hence,

$$\mathbf{u}\cdot\mathbf{n} \;=\; \frac{1}{k(x)}P_0(x,t) + \frac{1}{b(x)}\mathfrak{p}_{r(x)}[P_0](x,t)\,.$$

Elastoplastic boundary III

The Gauss formula yields again

$$U_\Omega(t) := \int_\Omega \operatorname{div} \mathbf{u} \, \mathrm{d}x \; = \; \int_{\partial\Omega} \Big(\frac{1}{k(x)} P_0(x,t) + \frac{1}{b(x)} \mathfrak{p}_{r(x)}[P_0](x,t) \Big) \, \mathrm{d}s(x) \, ,$$

Elastoplastic boundary III

The Gauss formula yields again

$$U_\Omega(t) := \int_\Omega \operatorname{div} \mathbf{u} \, \mathrm{d}x \;=\; \int_{\partial\Omega} \Big(\frac{1}{k(x)} P_0(x,t) + \frac{1}{b(x)} \mathfrak{p}_{r(x)}[P_0](x,t) \Big) \, \mathrm{d}s(x) \, ,$$

The mapping

$$\mathcal{F}[P](t) := \int_{\partial\Omega} \Big(\frac{1}{k(x)} P_0(x,t) + \frac{1}{b(x)} \mathfrak{p}_{r(x)}[P_0](x,t) \Big) \, \mathrm{d}s(x)$$

is the Prandtl-Ishlinskii hysteresis operator,

Elastoplastic boundary III

The Gauss formula yields again

$$U_\Omega(t) := \int_\Omega \mathrm{div}\,\mathbf{u}\,\mathrm{d}x \;=\; \int_{\partial\Omega} \Big(\frac{1}{k(x)} P_0(x,t) + \frac{1}{b(x)} \mathfrak{p}_{r(x)}[P_0](x,t)\Big)\,\mathrm{d}s(x)\,,$$

The mapping

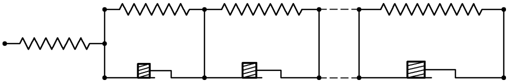
$$\mathcal{F}[P](t) := \int_{\partial\Omega} \Big(\frac{1}{k(x)} P_0(x,t) + \frac{1}{b(x)} \mathfrak{p}_{r(x)}[P_0](x,t)\Big)\,\mathrm{d}s(x)$$

is the Prandtl-Ishlinskii hysteresis operator, and the mechanical equilibrium reads

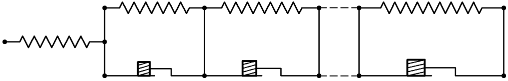
$$\nu U_t = -\lambda(U - \alpha(1-\chi)) + \beta(\theta - \theta_c) + \varrho_0 g x_3 - \mathcal{F}^{-1}[U_\Omega]\,.$$

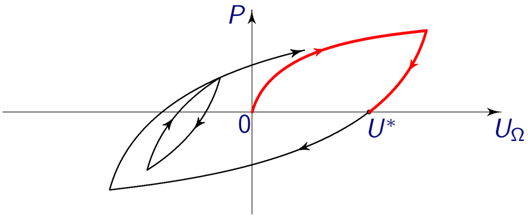
Note that the inverse $\mathcal{F}^{-1}$ is also a Prandtl-Ishlinskii operator.

The Prandtl-Ishlinskii operator



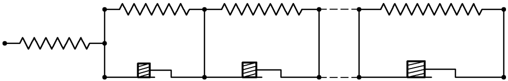
The Prandtl-Ishlinskii operator

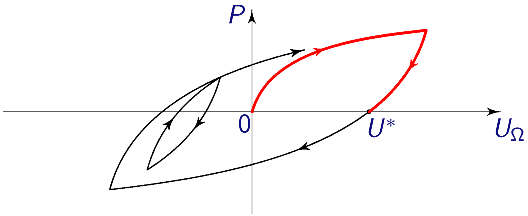




A diagram of the inverse Prandtl-Ishlinskii operator $\mathcal{F}^{-1}$.

The Prandtl-Ishlinskii operator





A diagram of the inverse Prandtl-Ishlinskii operator $\mathcal{F}^{-1}$.

When the pressure P increases from zero to some maximal value and then decreases to zero again (the red part of the diagram), a remanent volume deformation U^* persists in mechanical equilibrium.

Boundary condition for temperature

In the rigid or elastic case, no energy is dissipated on the boundary and we choose the boundary condition for θ as

$$\kappa(\chi)\nabla\theta \cdot \mathbf{n} + h(x)(\theta - \theta_\Gamma(x,t)) = 0$$

with given external temperature $\theta_\Gamma(x,t)$ and heat transfer coefficient $h(x) > 0$.

Boundary condition for temperature

In the rigid or elastic case, no energy is dissipated on the boundary and we choose the boundary condition for θ as

$$\kappa(\chi)\nabla\theta \cdot \mathbf{n} + h(x)(\theta - \theta_\Gamma(x,t)) = 0$$

with given external temperature $\theta_\Gamma(x,t)$ and heat transfer coefficient $h(x) > 0$.

If the boundary is elastoplastic, then the plastic dissipation appears as a boundary heat source

$$\kappa(\chi)\nabla\theta \cdot \mathbf{n} + h(x)(\theta - \theta_\Gamma) = \frac{r(x)}{b(x)}\left|\mathfrak{p}_{r(x)}[P_0]_t\right|$$

in the energy balance.

Mathematical results for the full model

Mathematical results for the full model

Derivation of the model, equilibria: PK + ER + JS, Wilmański Anniversary Volume, 2010.

Mathematical results for the full model

Derivation of the model, equilibria: PK + ER + JS, Wilmański Anniversary Volume, 2010.

We have shown that in "standard" containers (height less than a few kilometers, and a reasonable topological structure), there exists a unique equilibrium: Pure water for high temperatures, ice for low temperatures, or a sharp horizontal interface between ice (above) and water (below) for intermediate outer temperatures.

Mathematical results for the full model

Derivation of the model, equilibria: PK + ER + JS, Wilmański Anniversary Volume, 2010.

We have shown that in "standard" containers (height less than a few kilometers, and a reasonable topological structure), there exists a unique equilibrium: Pure water for high temperatures, ice for low temperatures, or a sharp horizontal interface between ice (above) and water (below) for intermediate outer temperatures.

Global existence and uniqueness for the elastic case under further assumptions: PK + ER, Frémond Anniversary Volume, 2013 (?)

Mathematical results for the full model

Derivation of the model, equilibria: PK + ER + JS, Wilmański Anniversary Volume, 2010.

We have shown that in "standard" containers (height less than a few kilometers, and a reasonable topological structure), there exists a unique equilibrium: Pure water for high temperatures, ice for low temperatures, or a sharp horizontal interface between ice (above) and water (below) for intermediate outer temperatures.

Global existence and uniqueness for the elastic case under further assumptions: PK + ER, Frémond Anniversary Volume, 2013 (?)

Main hypothesis: $\lim_{\theta \to \infty} \frac{c_1(\theta)}{\theta} = \infty$.

Mathematical results for the full model

Derivation of the model, equilibria: PK + ER + JS, Wilmański Anniversary Volume, 2010.

We have shown that in "standard" containers (height less than a few kilometers, and a reasonable topological structure), there exists a unique equilibrium: Pure water for high temperatures, ice for low temperatures, or a sharp horizontal interface between ice (above) and water (below) for intermediate outer temperatures.

Global existence and uniqueness for the elastic case under further assumptions: PK + ER, Frémond Anniversary Volume, 2013 (?)

Main hypothesis: $\lim_{\theta\to\infty} \frac{c_1(\theta)}{\theta} = \infty$.

Recall:

$$e_1(\theta) = \int_0^\theta c_1(\tau)\,\mathrm{d}\tau\,,\ \ s_1(\theta) = \int_0^\theta \frac{c_1(\tau)}{\tau}\,\mathrm{d}\tau\,,\ \ f_1(\theta) = e_1(\theta) - \theta s_1(\theta)\,.$$

Global solutions

For given initial conditions $\theta^0, U^0, \chi^0 \in L^\infty(\Omega)$, $\theta^0 \in H^1(\Omega)$, $\theta^0(x) \geq \theta_* > 0$, $\chi^0(x) \in [0, 1]$ a.e., we solve the system:

Global solutions

For given initial conditions $\theta^0, U^0, \chi^0 \in L^\infty(\Omega)$, $\theta^0 \in H^1(\Omega)$, $\theta^0(x) \geq \theta_* > 0$, $\chi^0(x) \in [0,1]$ a.e., we solve the system:

$$c(\chi)e_1(\theta)_t - \mathrm{div}\,(\kappa(\chi)\nabla\theta) = c'(\chi)\chi_t(f_1(\theta) - e_1(\theta))$$

$$+\nu U_t^2 - \beta\theta U_t + \gamma\chi_t^2 - L\frac{\theta}{\theta_c}\chi_t\,,$$

Global solutions

For given initial conditions $\theta^0, U^0, \chi^0 \in L^\infty(\Omega)$, $\theta^0 \in H^1(\Omega)$, $\theta^0(x) \geq \theta_* > 0$, $\chi^0(x) \in [0,1]$ a.e., we solve the system:

$$
\begin{aligned}
c(\chi)e_1(\theta)_t - \mathrm{div}\,(\kappa(\chi)\nabla\theta) &= c'(\chi)\chi_t(f_1(\theta) - e_1(\theta)) \\
&\quad + \nu U_t^2 - \beta\theta U_t + \gamma\chi_t^2 - L\frac{\theta}{\theta_c}\chi_t\,, \\
\nu U_t + \lambda(\chi)(U - \alpha(1-\chi)) - \beta(\theta - \theta_c) &= \varrho_0 g x_3 - K_\Gamma \int_\Omega U\,\mathrm{d}x - \tilde{P}(t)\,,
\end{aligned}
$$

Global solutions

For given initial conditions $\theta^0, U^0, \chi^0 \in L^\infty(\Omega)$, $\theta^0 \in H^1(\Omega)$, $\theta^0(x) \geq \theta_* > 0$, $\chi^0(x) \in [0,1]$ a.e., we solve the system:

$$
\begin{aligned}
c(\chi)e_1(\theta)_t - \mathrm{div}\,(\kappa(\chi)\nabla\theta) &= c'(\chi)\chi_t(f_1(\theta) - e_1(\theta)) \\
&\quad + \nu U_t^2 - \beta\theta U_t + \gamma\chi_t^2 - L\frac{\theta}{\theta_c}\chi_t\,, \\
\nu U_t + \lambda(\chi)(U - \alpha(1-\chi)) - \beta(\theta - \theta_c) &= \varrho_0 g x_3 - K_\Gamma \int_\Omega U\,\mathrm{d}x - \tilde{P}(t)\,, \\
-\gamma\chi_t - \frac{\lambda'(\chi)}{2}(U - \alpha(1-\chi))^2 &- \alpha\lambda(\chi)(U - \alpha(1-\chi)) \\
&\in c'(\chi)\,(f_1(\theta) - f_1(\theta_c)) + L\left(1 - \frac{\theta}{\theta_c}\right) + \partial I(\chi)\,.
\end{aligned}
$$

Global solutions II

The main difficulty comes from the quadratic term in the phase evolution equation.

- For a cut-off system, existence and uniqueness on every time interval $(0, T)$ are obtained for a time semidiscrete system;

Global solutions II

The main difficulty comes from the quadratic term in the phase evolution equation.

- For a cut-off system, existence and uniqueness on every time interval $(0, T)$ are obtained for a time semidiscrete system;
- Energy + entropy estimates enable us to let the discretization parameter tend to zero and obtain a solution to the cut-off system;

Global solutions II

The main difficulty comes from the quadratic term in the phase evolution equation.

- For a cut-off system, existence and uniqueness on every time interval $(0, T)$ are obtained for a time semidiscrete system;
- Energy + entropy estimates enable us to let the discretization parameter tend to zero and obtain a solution to the cut-off system;
- Uniform bounds independent of the cut-off parameter follow from Moser-Alikakos iterations;

Global solutions II

The main difficulty comes from the quadratic term in the phase evolution equation.

- For a cut-off system, existence and uniqueness on every time interval $(0, T)$ are obtained for a time semidiscrete system;
- Energy + entropy estimates enable us to let the discretization parameter tend to zero and obtain a solution to the cut-off system;
- Uniform bounds independent of the cut-off parameter follow from Moser-Alikakos iterations;
- Uniqueness of the solution is obtained if the heat conductivity κ is constant.

Cut-off

Cut-off

We introduce, for $\theta \in \mathbb{R}$, $R > 0$, the functions

$$Q_R(\theta) = \min\{\theta^+, B(R)\}, \quad B(R) = R^{1/2}(\min\{e_1(R), |f_1(R)|\})^{1/4},$$
$$c_1^R(\theta) = c_1(Q_R(\theta)),$$
$$e_1^R(\theta) = \int_0^\theta c_1^R(\tau)\,\mathrm{d}\tau,$$
$$s_1^R(\theta) = \int_0^\theta \frac{c_1^R(\tau)}{Q_R(\tau)}\,\mathrm{d}\tau,$$
$$f_1^R(\theta) = e_1^R(\theta) - Q_R(\theta)s_1^R(\theta) = \int_0^\theta c_1^R(\tau)\left(1 - \frac{Q_R(\theta)}{Q_R(\tau)}\right)\mathrm{d}\tau,$$

Cut-off

We introduce, for $\theta \in \mathbb{R}$, $R > 0$, the functions

$$Q_R(\theta) = \min\{\theta^+, B(R)\}, \quad B(R) = R^{1/2}(\min\{e_1(R), |f_1(R)|\})^{1/4},$$
$$c_1^R(\theta) = c_1(Q_R(\theta)),$$
$$e_1^R(\theta) = \int_0^\theta c_1^R(\tau)\,\mathrm{d}\tau,$$
$$s_1^R(\theta) = \int_0^\theta \frac{c_1^R(\tau)}{Q_R(\tau)}\,\mathrm{d}\tau,$$
$$f_1^R(\theta) = e_1^R(\theta) - Q_R(\theta)s_1^R(\theta) = \int_0^\theta c_1^R(\tau)\left(1 - \frac{Q_R(\theta)}{Q_R(\tau)}\right)\mathrm{d}\tau,$$

Main property:

$$\lim_{R\to\infty} \frac{e_1(R)}{B^2(R)} = \lim_{R\to\infty} \frac{B(R)}{R} = \infty.$$

Energy + entropy bound

Energy + entropy bound

For the "extended" energy $\varrho_0(e - \bar{\theta}_\Gamma s)$, with some fixed constant temperature $\bar{\theta}_\Gamma$, we have the following balance equation:

$$
\begin{aligned}
&\int_\Omega \left(c(\chi)(e_1(\theta) - f_1(\theta_c)) + \frac{\lambda(\chi)}{2}(U - \alpha(1-\chi))^2 \right)(x,t)\,\mathrm{d}x \\
&\quad + \int_\Omega (\beta\theta_c U + L\chi - \varrho_0 g x_3 U)(x,t)\,\mathrm{d}x \\
&\quad + \frac{K_\Gamma}{2}\left(U_\Omega(t) + P_0(t) + \frac{\varrho_0 g\,\zeta_\Gamma}{K_\Gamma} \right)^2 \\
&\quad + \bar{\theta}_\Gamma \int_0^t \int_\Omega \left(\frac{\kappa(\chi)|\nabla\theta|^2}{\theta^2} + \frac{\gamma(\theta)}{\theta}\chi_t^2 + \frac{\nu}{\theta}U_t^2 \right)(x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi \\
&\quad + \int_0^t \int_{\partial\Omega} \frac{h(x)}{\theta}(\theta - \theta_\Gamma(x,\xi))(\theta - \bar{\theta}_\Gamma)\,\mathrm{d}\sigma(x)\,\mathrm{d}\xi \\
= \; & E^0 + E^0_\Gamma - \bar{\theta}_\Gamma S^0 + \bar{\theta}_\Gamma \int_\Omega \left(c(\chi)s_1(\theta) + \frac{L}{\theta_c}\chi + \beta U \right)(x,t)\,\mathrm{d}x \\
&\quad + \int_0^t K_\Gamma (P_0)_t(\xi) \left(U_\Omega(\xi) + P_0(\xi) + \frac{\varrho_0 g \zeta_\Gamma}{K_\Gamma} \right) \mathrm{d}\xi\,.
\end{aligned}
$$

Moser-Alikakos iterations

Moser-Alikakos iterations

The truncated energy balance

$$
\begin{aligned}
c(\chi) e_1^R(\theta)_t - \mathrm{div}\,(\kappa(\chi)\nabla\theta) \;&=\; c'(\chi)\chi_t(f_1^R(\theta) - e_1^R(\theta)) \\
&+ \nu U_t^2 - \beta Q_R(\theta) U_t + \gamma \chi_t^2 - L \frac{Q_R(\theta)}{\theta_c}\chi_t
\end{aligned}
$$

Moser-Alikakos iterations

The truncated energy balance

$$\begin{aligned} c(\chi)e_1^R(\theta)_t - \operatorname{div}(\kappa(\chi)\nabla\theta) &= c'(\chi)\chi_t(f_1^R(\theta) - e_1^R(\theta)) \\ &\quad + \nu U_t^2 - \beta Q_R(\theta)U_t + \gamma\chi_t^2 - L\frac{Q_R(\theta)}{\theta_c}\chi_t \end{aligned}$$

is tested by v^p, letting $p \to \infty$, with a clever choice of v,

Moser-Alikakos iterations

The truncated energy balance

$$
\begin{aligned}
c(\chi)e_1^R(\theta)_t - \mathrm{div}\,(\kappa(\chi)\nabla\theta) \;&=\; c'(\chi)\chi_t(f_1^R(\theta) - e_1^R(\theta)) \\
&\quad + \nu U_t^2 - \beta Q_R(\theta) U_t + \gamma\chi_t^2 - L\frac{Q_R(\theta)}{\theta_c}\chi_t
\end{aligned}
$$

is tested by v^p, letting $p \to \infty$, with a clever choice of v,

$$
v = (Q_R(\theta) - R)^+ .
$$

Moser-Alikakos iterations

The truncated energy balance

$$c(\chi)e_1^R(\theta)_t - \mathrm{div}\,(\kappa(\chi)\nabla\theta) \;=\; c'(\chi)\chi_t(f_1^R(\theta) - e_1^R(\theta)) + \nu U_t^2 - \beta Q_R(\theta) U_t + \gamma\chi_t^2 - L\frac{Q_R(\theta)}{\theta_c}\chi_t$$

is tested by v^p, letting $p \to \infty$, with a clever choice of v,

$$v = (Q_R(\theta) - R)^+ .$$

The right hand side can be rewritten as a sum of one bounded term with a product of two terms of opposite signs provided R is sufficiently large.

Conclusions

Conclusions

- A simple 3D model is proposed for mechanical interaction between a substance undergoing phase transition and the boundary of the container;

Conclusions

- A simple 3D model is proposed for mechanical interaction between a substance undergoing phase transition and the boundary of the container;
- The pressure due to freezing may become by three orders of magnitude higher than the standard pressure;

Conclusions

- A simple 3D model is proposed for mechanical interaction between a substance undergoing phase transition and the boundary of the container;
- The pressure due to freezing may become by three orders of magnitude higher than the standard pressure;
- Although the gravity force in small containers ($< 1\,\mathrm{m}$) is by four orders of magnitude weaker than pressure forces, it has a substantial qualitative influence on the long time behavior by selecting a unique equilibrium with solid on the top and liquid on the bottom;

Conclusions

- A simple 3D model is proposed for mechanical interaction between a substance undergoing phase transition and the boundary of the container;
- The pressure due to freezing may become by three orders of magnitude higher than the standard pressure;
- Although the gravity force in small containers ($< 1\,\mathrm{m}$) is by four orders of magnitude weaker than pressure forces, it has a substantial qualitative influence on the long time behavior by selecting a unique equilibrium with solid on the top and liquid on the bottom;
- Elastoplastic response of the container is manifested by the occurrence of hysteresis operators in the mechanical balance equation, and as a boundary heat source in the energy balance equation.

Conclusions

- A simple 3D model is proposed for mechanical interaction between a substance undergoing phase transition and the boundary of the container;
- The pressure due to freezing may become by three orders of magnitude higher than the standard pressure;
- Although the gravity force in small containers ($< 1\,\mathrm{m}$) is by four orders of magnitude weaker than pressure forces, it has a substantial qualitative influence on the long time behavior by selecting a unique equilibrium with solid on the top and liquid on the bottom;
- Elastoplastic response of the container is manifested by the occurrence of hysteresis operators in the mechanical balance equation, and as a boundary heat source in the energy balance equation.
- The solutions to the full evolution system can be constructed by time semidiscretization, cut-off and Moser-Alikakos iterations.

Conclusions

- A simple 3D model is proposed for mechanical interaction between a substance undergoing phase transition and the boundary of the container;
- The pressure due to freezing may become by three orders of magnitude higher than the standard pressure;
- Although the gravity force in small containers ($< 1\,\mathrm{m}$) is by four orders of magnitude weaker than pressure forces, it has a substantial qualitative influence on the long time behavior by selecting a unique equilibrium with solid on the top and liquid on the bottom;
- Elastoplastic response of the container is manifested by the occurrence of hysteresis operators in the mechanical balance equation, and as a boundary heat source in the energy balance equation.
- The solutions to the full evolution system can be constructed by time semidiscretization, cut-off and Moser-Alikakos iterations.
- The long time asymptotics of the trajectories has been studied in special cases only.