Coupled Thermomechanical Contact Problems
Computational Modeling of Solidification Processes

C. Agelet de Saracibar, M. Chiumenti, M. Cervera
ETS Ingenieros de Caminos, Canales y Puertos, Barcelona, UPC
International Center for Numerical Methods in Engineering (CIMNE)

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Outline

Motivation and Goals
Coupled Thermomechanical Problem
Mechanical Problem
  Solid Phase
  Liquid Phase
  Mushy Zone. Liquid-Solid Continuous Transition
  Multigrid Scale Pressure Stabilization
Thermal Problem
Mechanical Contact Problem
Thermal Contact Problem
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Concluding Remarks
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Motivation and Goals

Truthful coupled thermomechanical simulation of solidification and cooling processes of industrial cast parts (usually meaning complex geometries), in particular for aluminium alloys in permanent moulds.

Thermodynamically consistent material model allowing a continuous transition between the different states of the process, from an initial fully liquid state to a final fully solid state.

Thermomechanical contact model allowing the simulation of the interaction among all casting tools as consequence of the thermal deformations generated by high temperature gradients and phase transformations during solidification and cooling processes.

Suitable stable FE formulation for linear tetrahedral elements, which allow the FE discretization of complex industrial geometries, and for incompressible or quasi-incompressible problems.
Motivation and Goals
Motivation and Goals
Outline

Motivation and Goals

**Coupled Thermomechanical Problem**

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Thermal Contact Problem

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Coupled Thermomechanical Problem
Fractional Step Method, Product Formula Algorithm

LOOP, TIME

Solve the THERMAL PROBLEM at constant configuration
Solve the discrete variational form of the energy balance equation

\[
(C \dot{\Theta} + \dot{L}, \delta \Theta) + (K \nabla \Theta, \nabla \delta \Theta) = -(\overline{Q}, \delta \Theta)_{\partial \Omega_Q} - (Q_c, \delta \Theta)_{\partial \Omega_{tc}}
\]

Obtain the temperatures map

Solve the MECHANICAL PROBLEM at constant temperature
Solve the discrete variational form of the momentum balance equation

\[
(\sigma, \nabla^s \delta u) = (B, \delta u) + (t, \delta u)_{\partial \Omega_{\sigma}} + (\overline{t}, \delta u)_{\partial \Omega_{mc}}
\]

Obtain the displacements map, and then the stresses map

END LOOP, TIME
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Coupled Thermomechanical Problem

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Solid and Liquid-like Phases
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Solid and Liquid-like Phases
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Mechanical Problem
Solid Phase

Prof. Dr. Ing. Carlos Agelet de Saracibar
J2 Elasto-Viscoplastic model, isotropic and kinematic hardening

The thermoelastic constitutive behaviour in solid state \((\Theta \leq \Theta_S)\) can be written as,

\[
p = K(\Theta)(\nabla \cdot \mathbf{u} - e^\Theta)
\]

\[
s = 2G(\Theta)\text{dev}\left(\varepsilon - \varepsilon^p\right)
\]

where the \(p\) is the mean pressure, \(s\) is the deviatoric part of the stress tensor, \(K(\Theta)\) is the bulk modulus, \(G(\Theta)\) is the shear modulus \(e^\Theta\) and is the volumetric thermal deformation which takes also into account the thermal shrinkage due to phase-change,

\[
e^\Theta \Theta = 1 - \frac{\rho_L}{\rho_S} + 3\alpha (\Theta - \Theta_{\text{ref}}) - 3\alpha (\Theta_S - \Theta_{\text{ref}})
\]
Mechanical Problem
Solid Phase

**J2 Elasto-Viscoplastic model, isotropic and kinematic hardening**

The *yield function* can be written as,

\[ \Phi(s, q, q, \Theta) := \| s - q \| - R(q, \Theta) \]

where the *yield radius* takes the form,

\[ R(q, \Theta) = \sqrt{\frac{2}{3}} \left( \sigma_0(\Theta) - q \right) \]
J2 Elasto-Viscoplastic model, isotropic and kinematic hardening

The plastic evolution equations can be written as,

\[ \dot{\varepsilon}^p = \gamma \partial_\sigma \Phi(s, q, q, \Theta) = \gamma n \]

\[ \dot{\xi} = \gamma \partial_q \Phi(s, q, q, \Theta) = \gamma \sqrt{2/3} \]

\[ \dot{\xi} = -\gamma n \]

where the plastic parameter takes the form,

\[ \gamma = \frac{1}{\eta} \langle \Phi(s, q, q, \Theta) \rangle^n \]

and the unit normal to the yield surface takes the form,

\[ n = (s - q)/\|s - q\| \]
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Liquid-like Phase

Viscous deviatoric model

In the liquid state \((\Theta \geq \Theta_L)\), the thermal deformation is zero and the bulk modulus and shear modulus tends to infinity, characterizing an incompressible rigid-plastic material, such that

\[
e^\Theta(\Theta) = 0, \quad K(\Theta) \to \infty \quad \Rightarrow \quad \nabla \cdot \mathbf{u} = 0
\]

\[
G(\Theta) \to \infty \quad \Rightarrow \quad \mathbf{\varepsilon} := \mathbf{\varepsilon}^p, \quad \mathbf{\varepsilon}^e = 0
\]

A purely viscous deviatoric model can be obtained as a particular case of the J2 elasto-viscoplastic model, without considering neither isotropic or kinematic hardening and setting to zero the radius of the yield surface. Then the yield function takes the form,

\[
\Phi(s) := \|s\|
\]
Mechanical Problem
Liquid-like Phase

Viscous deviatoric model

The plastic evolution equation takes the form,

$$\dot{\mathbf{e}}^p = \gamma \partial_\sigma \Phi(s) = \gamma \mathbf{n}$$

where the plastic parameter and unit normal to the yield surface take the form,

$$\gamma = \frac{1}{\eta} \langle \Phi(s) \rangle \quad \mathbf{n} = \mathbf{s}/\|s\|$$

and the plastic strain evolution takes the simple form,

$$\dot{\mathbf{e}}^p = \frac{1}{\eta} \mathbf{s}$$
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**Mechanical Problem**

*Mushy Zone. Liquid-Solid Continuous Transition*

**J2 Elasto-Viscoplastic model, isotropic and kinematic hardening**

The **thermoelastic constitutive behaviour in mushy state** \((\Theta_L < \Theta < \Theta_S)\) can be written as,

\[
p = K(\Theta)(\nabla \cdot \mathbf{u} - e^\theta) \\
s = 2G(\Theta)\text{dev}(\mathbf{\varepsilon} - \mathbf{\varepsilon}^p)
\]

where the \(p\) is the mean pressure, \(s\) is the deviatoric part of the stress tensor, \(K(\Theta)\) is the bulk modulus, \(G(\Theta)\) is the shear modulus \(e^\theta\) and is the volumetric thermal deformation due to the thermal shrinkage taking place during the liquid-solid phase-change,

\[
e^\theta \Theta = \frac{\Delta V^{pc}}{V_0} f_S \Theta = \frac{\rho \Theta - \rho_L}{\rho_S}
\]
Mechanical Problem
Mushy Zone. Liquid-Solid Continuous Transition

**J2 Elasto-Viscoplastic model, isotropic and kinematic hardening**

The yield function can be written as,

\[
\Phi(s, q, q, \Theta) := \left\| s - f_s(\Theta)q \right\| - f_s(\Theta)R(q, \Theta)
\]

where the solid fraction satisfies,

\[
f_s(\Theta) = 0 \quad \Theta_L \leq \Theta
\]

\[
f_s(\Theta) = 1 \quad \Theta \leq \Theta_S
\]

The yield function for the solid phase is recovered for \( f_s(\Theta) = 1 \)

The yield function for the liquid-like phase is recovered for \( f_s(\Theta) = 0 \)
J2 Elasto-Viscoplastic model, isotropic and kinematic hardening

The plastic evolution equations can be written as,

\[ \dot{\varepsilon}^p = \gamma \partial_\sigma \Phi(s, q, q, \Theta) = \gamma n \]

\[ \dot{\varepsilon}^{\|} = \gamma \partial_q \Phi(s, q, q, \Theta) = \gamma \sqrt{2/3} f_s(\Theta) \]

\[ \dot{\varepsilon}^{\perp} = \gamma \partial_{\theta} \Phi(s, q, q, \Theta) = -\gamma n f_s(\Theta) \]

where the plastic parameter takes the form,

\[ \gamma = \frac{1}{\eta} \langle \Phi(s, q, q, \Theta) \rangle^n \]

and the unit normal to the yield surface takes the form,

\[ n = \left( s - f_s(\Theta)q \right) / \| s - f_s(\Theta)q \| \]
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Incompressibility or Quasi-incompressibility Problem

Low order standard finite elements discretizations are very convenient for the numerical simulation of large scale complex industrial casting problems:

- Relatively easy to generate for real life complex geometries
- Computational efficiency
- Well suited for contact problems

Low order standard finite elements lock for incompressible or quasi-incompressible problems.

Mixed u/p finite element formulations may avoid this locking behaviour, but they must satisfy a pressure stability restriction on the interpolation degree for the u/p fields given by the Babuska-Brezzi pressure stability condition.

Finite elements based on equal u/p finite element interpolation order do not satisfy the BB stability condition. Standard mixed linear/linear u/p triangles or tetrahedra elements do not satisfy the BB stability condition, exhibiting spurious pressure oscillations.
Mechanical Problem
Incompressibility or Quasi-incompressibility Problem

Pressure stabilization goals

To stabilize the pressure while using mixed equal order linear $u/p$ triangles and tetrahedra

Stabilization of incompressibility or quasi-incompressibility problems using Orthogonal Subgrid Scale Method, within the framework of Variational Multiscale Methods (Hughes, 1995; Garikipati & Hughes, 1998, 2000; Codina, 2000, 2002; Chiumenti et al. 2002, 2004; Cervera et al. 2003; Agelet de Saracibar et al. 2006)
Mechanical Problem
Incompressibility or Quasi-incompressibility Problem

Pressure map

P1
Standard Galerkin linear u
element

P1/P1
Standard mixed linear/linear u/p
element

P1/P1 OSGS
Stabilized mixed linear u/p
element
Mechanical Problem
Multiscale Stabilization Methods

Strong form of the mixed quasi-incompressible problem

Let us consider the following infinite-dimensional spaces for the displacements and pressure fields, respectively,

$$
\mathcal{V} := \left\{ \mathbf{u} \in H^1(\Omega) \left| \mathbf{u} = \mathbf{u}_0 \quad \text{on} \quad \partial_u \Omega \right. \right\} \quad \mathcal{Q} := L^2(\Omega)
$$

Find a displacement field $\mathbf{u} \in \mathcal{V}$ and pressure field $p \in \mathcal{Q}$ such that,

$$
\begin{align*}
\nabla \cdot \mathbf{s} + \nabla p + \mathbf{B} &= 0 \\
\nabla \cdot \mathbf{u} - e^\theta - \frac{1}{K} p &= 0
\end{align*}
$$

in $\Omega$

Find $\mathbf{U} \in \mathcal{W} := \mathcal{V} \times \mathcal{Q}$ such that,

$$
\mathcal{L}(\mathbf{U}) = \mathbf{F} \quad \text{in} \ \Omega
$$
Mechanical Problem
Multiscale Stabilization Methods

Variational form of the mixed quasi-incompressible problem

Let us consider the following infinite-dimensional spaces for the displacements, displacements variations and pressure fields, respectively,

\[ \mathcal{V} := \left\{ \mathbf{u} \in H^1(\Omega) \mid \mathbf{u} = \mathbf{u}_0 \text{ on } \partial_u \Omega \right\} \quad \mathcal{V}_o := H^1_0(\Omega) \quad \mathcal{Q} := L^2(\Omega) \]

Find a displacement field \( \mathbf{u} \in \mathcal{V} \) and pressure field \( p \in \mathcal{Q} \) such that,

\[
\begin{aligned}
\left( s, \nabla^s \mathbf{v} \right) + \left( p, \nabla \cdot \mathbf{v} \right) - \left( \mathbf{B}, \mathbf{v} \right) - \left( \mathbf{t}, \mathbf{v} \right)_{\partial \Omega} &= 0 \quad \forall \mathbf{v} \in \mathcal{V}_o \\
\left( \nabla \cdot \mathbf{u} - e^\theta, q \right) - \frac{1}{K} \left( p, q \right) &= 0 \quad \forall q \in \mathcal{Q}
\end{aligned}
\]

Find \( \mathbf{U} \in \mathcal{W} := \mathcal{V} \times \mathcal{Q} \) such that,

\[
B(\mathbf{U}, \mathbf{V}) = L(\mathbf{V}) \quad \forall \mathbf{V} \in \mathcal{W}_o := \mathcal{V}_o \times \mathcal{Q} \quad \text{in } \Omega
\]
Mechanical Problem
Multiscale Stabilization Methods

Multiscale methods. Subgrid multiscale technique

Let us consider the following \textit{split} of the exact solution field,

\[ U := U_h + \tilde{U} \in \mathcal{W} := \mathcal{V} \times \mathcal{Q} \]

where \( U \) is the \textit{exact solution}, \( U_h \in \mathcal{W}_h = \mathcal{V}_h \times \mathcal{Q}_h \) is the \textit{finite element approximated solution} (belonging to the finite-dimensional FE solution space) and \( \tilde{U} \in \tilde{\mathcal{W}} = \tilde{\mathcal{V}} \times \tilde{\mathcal{Q}} \) is the \textit{subgrid scale solution}, not captured by the finite element mesh, belonging to the infinite-dimensional subgrid scale space

\[
U = \begin{bmatrix} u \\ p \end{bmatrix}, \quad U_h = \begin{bmatrix} u_h \\ p_h \end{bmatrix}, \quad \tilde{U} = \begin{bmatrix} \tilde{u} \\ 0 \end{bmatrix}
\]
Orthogonal Subgrid Scale (OSGS) technique

Within the OSGS technique, the infinite-dimensional subgrid scale space is approximated by a finite-dimensional space chosen to be orthogonal to the FE solution space (Codina, 2000)

\[ \tilde{U} \in \tilde{W} \approx \mathcal{W}_h^\perp \]
Mechanical Problem  
OSGS Stabilization Technique

Orthogonal Subgrid Scale (OSGS) technique

The subgrid scale solution is then approximated, at the element level as,

\[
\tilde{\mathbf{u}}_{n+1} = \tau_{e,n+1} P_{h}^{\perp} \left( \nabla \cdot \mathbf{s}_{h,n+1} + \nabla P_{h,n+1} + \mathbf{B} \right)
\]

\[
\tilde{p}_{n+1} = 0
\]

where \( \tau_{e,n+1} \) is a (mesh size dependent) stabilization parameter defined as,

\[
\tau_{e,n+1} = \frac{c h_e^2}{2G^*}
\]

where \( G^* \) is the secant shear modulus.
Orthogonal Subgrid Scale (OSGS) technique

Using a linear interpolation for displacements (triangles/tetrahedra) and assuming that body forces belong to the FE space, the subgrid scale solution is then approximated, at the element level as,

$$\tilde{u}_{n+1} = \tau_{e,n+1} P_h^\perp \left( \nabla p_{h,n+1} \right)$$

$$\tilde{p}_{n+1} = 0$$

where $\tau_{e,n+1}$ is a (mesh size dependent) stabilization parameter defined as,

$$\tau_{e,n+1} = \frac{c h_e^2}{2 G^*}$$

where $G^*$ is the secant shear modulus.
Mechanical Problem
OSGS Stabilization Technique

Discrete OSGS stabilized variational form

Find $\mathbf{U}_h \in \mathcal{W}_h$ such that, for any $\mathbf{V}_h \in \mathcal{W}_{0,h}$

$$B_{stab}(\mathbf{U}_h, \mathbf{V}_h) = L_{stab}(\mathbf{V}_h) \quad \forall \mathbf{V}_h \in \mathcal{W}_{0,h}$$

where the stabilized variational forms can be written as,

$$B_{stab}(\mathbf{U}_h, \mathbf{V}_h) = B(\mathbf{U}_h, \mathbf{V}_h) - \sum_{e=1}^{n_{elem}} \left( \tau_{e,n+1} P_{h}^\perp \left( \nabla p_{h,n+1} \right), \nabla q_h \right)_{\Omega_e}$$

$$L_{stab}(\mathbf{V}_h) = L(\mathbf{V}_h)$$
Mechanical Problem
OSGS Stabilization Technique

Discrete OSGS stabilized variational form

Let $\Pi_{h,n+1} := P_h \left( \nabla p_{h,n+1} \right)$ the projection of the discrete pressure gradient onto the FE solution space and $\mathcal{V} = H^1, \mathcal{V}_h \subset \mathcal{V}$ the pressure gradient projection and FE associated spaces, respectively.

Then the orthogonal projection of the discrete pressure gradient onto the FE solution space takes the form,

$$P_h \perp \left( \nabla p_{h,n+1} \right) = \nabla p_{h,n+1} - \Pi_{h,n+1}$$
Mechanical Problem
OSGS Stabilization Technique

Discrete OSGS stabilized variational form

Find \( \{ u_{h,n+1}, p_{h,n+1}, \Pi_{h,n+1} \} \in \mathcal{V}_h \times \mathcal{Q}_h \times \mathcal{Y}_h \) such that,

\[
\begin{align*}
(s_{h,n+1}, \nabla_{n+1} v_h) + (p_{h,n+1}, \nabla_{n+1} \cdot v_h) - (B, v_h) - (t, v_h)_{\partial \Omega} = 0 \\
(\nabla_{n+1} \cdot u_{h,n+1}, q_h) - \frac{1}{K} (p_{h,n+1}, q_h) - \sum_{e=1}^{n_{\text{elem}}} (\tau_{e,n+1} (\nabla_{n+1} p_{h,n+1} - \Pi_{h,n+1}), \nabla_{n+1} q_h)_{\Omega_e} = 0 \\
(\nabla_{n+1} p_{h,n+1} - \Pi_{h,n+1}, \pi_h) = 0
\end{align*}
\]

for any \( \{ v_h, q_h, \pi_h \} \in \mathcal{V}_{h,0} \times \mathcal{Q}_h \times \mathcal{V}_{h,0} \)
Mechanical Problem
OSGS Stabilization Technique

Strong form of the stabilized mixed quasi-incompressible problem

Let us consider the following infinite-dimensional spaces for the displacements, pressure and pressure gradient projection fields, respectively,

\[ \mathcal{V} := \left\{ \mathbf{u} \in H^1(\Omega) \mid \mathbf{u} = \mathbf{\bar{u}} \text{ on } \partial_u \Omega \right\} \quad \mathcal{Q} := L^2(\Omega) \quad \mathcal{Y} = H^1(\Omega) \]

Find a displacement field \( \mathbf{u} \in \mathcal{V} \), a pressure field \( p \in \mathcal{Q} \) and a pressure gradient projection \( \Pi \in \mathcal{Y} \) such that,

\[ \begin{align*}
\nabla \cdot \mathbf{s} + \nabla p + \mathbf{B} &= 0 \\
\nabla \cdot \mathbf{u} - \frac{1}{K} p + \tau \left( \nabla^2 p - \nabla \cdot \Pi \right) &= 0 \quad \text{in } \Omega \\
\n\nabla p - \Pi &= 0
\end{align*} \]
Staggered solution procedure. Problem 1

Given \( \{ \Pi_{h,n} \} \in \Upsilon_h \) find \( \{ u_{h,n+1}, p_{h,n+1} \} \in V_h \times Q_h \) such that,

\[
\begin{align*}
\left( s_{h,n+1}, \nabla_{n+1}^s v_h \right) + \left( p_{h,n+1}, \nabla_{n+1} \cdot v_h \right) - \left( B, v_h \right) - \left( t, v_h \right)_{\partial_{\sigma} \Omega} &= 0 \\
\left( \nabla_{n+1} \cdot u_{h,n+1}, q_h \right) - \frac{1}{K} \left( p_{h,n+1}, q_h \right) - \sum_{e=1}^{n_{elem}} \left( \tau_{e,n}, \nabla_{n} p_{h,n+1} - \Pi_{h,n} \right), \nabla_{n} q_{h} \right)_{\Omega_e} &= 0
\end{align*}
\]

for any \( \{ v_h, q_h \} \in V_{h,0} \times Q_h \)
Staggered solution procedure. Problem 2

Given \( \{u_{h,n+1}, p_{h,n+1}\} \in \mathcal{V}_h \times \mathcal{Q}_h \) find \( \{\Pi_{h,n+1}\} \in \mathcal{Y}_h \) such that,

\[
\sum_{e=1}^{n_{\text{elem}}} \tau_{e,n+1} \left( \nabla_{n+1} p_{h,n+1} - \Pi_{h,n+1}, \pi_h \right)_{\Omega_e} = 0
\]

for any \( \{\pi_h\} \in \mathcal{V}_{h,0} \)
Mechanical Problem
OSGS Stabilization Technique

Matrix form of the staggered solution procedure

Problem 1. Solve the algebraic system of equations to compute the incremental discrete displacements and pressures unknowns

\[ K^{(i)}_{\tau,n+1} \Delta U_{n+1}^{(i)} + G^{(i)}_{n+1} \Delta P_{n+1}^{(i)} = -R_{u,n+1}^{(i)} \]

\[ G^{(i)T}_{n+1} \Delta U_{n+1}^{(i)} - (M_p + L_{\tau,n}) \Delta P_{n+1}^{(i)} = -R_{p,n+1}^{(i)} \]

Problem 2. Compute the discrete continuous pressure gradient projections unknowns

\[ \Pi_{n+1} = M_{\tau,n+1}^{-1} G_{\tau,n+1} P_{n+1} \]
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Energy Balance

Variational enthalpy form of energy balance

\[
\left( \dot{H}, \partial \Theta \right) + \left( K \nabla \Theta, \nabla \partial \Theta \right) = - \left( \bar{Q}, \partial \Theta \right)_{\partial \Omega_Q} - \left( Q_c, \partial \Theta \right)_{\partial \Omega_{lc}}
\]

where the enthalpy rate is given by,

\[
\dot{H} = C \dot{\Theta} + \dot{L}(\Theta)
\]

where the latent heat release is given by,

\[
\dot{L}(\Theta) = -L \frac{df_s}{d\Theta} \dot{\Theta} = L \frac{df_l}{d\Theta} \dot{\Theta}
\]

where the solid fraction satisfies,

\[
f_s(\Theta) = 0 \quad \Theta_L \leq \Theta
\]

\[
f_s(\Theta) = 1 \quad \Theta \leq \Theta_S
\]

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Nonlinear Contact Kinematics

Reference Configurations

$t = 0$

Master Body

$X^{(2)}$

$\Omega^{(2)}$

$\Gamma^{(2)}$

$N^{(2)}$

Slave Body

$X^{(1)}$

$\Omega^{(1)}$

$\Gamma^{(1)}$

Current Configurations

$t$

$\varphi_t^{(2)}$

$\varphi_t^{(1)}$

$\varphi^{(2)}(\Omega^{(2)})$

$\varphi^{(1)}(\Omega^{(1)})$

$\mathbf{x}^{(2)}(X^{(1)}, t) = \text{ARGMIN}_{\forall \mathbf{x}^{(2)} \in \Gamma^{(2)}} \left\{ \left\| \varphi_t^{(1)}(X^{(1)}) - \varphi_t^{(2)}(X^{(2)}) \right\| \right\}$

$\mathbf{x}^{(2)}(X^{(1)}, t) = \varphi_t^{(2)}(\bar{\mathbf{x}}^{(2)})$

$\mathbf{n}^{(1)}$

$\mathbf{n}^{(2)}$

$\gamma^{(1)}$

$\gamma^{(2)}$

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Nonlinear Contact Kinematics

Closest-Point-Projection onto the Master Surface

\[ \bar{X}^{(2)} \left( X^{(1)}, t \right) = \arg\min_{\forall \bar{X}^{(2)} \in \Gamma^{(2)}} \left\{ \left\| \varphi^{(1)}_t \left( X^{(1)} \right) - \varphi^{(2)}_t \left( X^{(2)} \right) \right\| \right\} \]

\[ \bar{x}^{(2)} \left( X^{(1)}, t \right) = \varphi^{(2)}_t \left( \bar{X}^{(2)} \left( X^{(1)}, t \right) \right) \]

\( X^{(1)} \) ... Coordinates of the slave particle at reference configuration

\( \bar{X}^{(2)} \) ... Coordinates of the master particle at reference configuration, defined as the closest-point-projection of the slave particle onto the master surface at the current configuration

\( \bar{x}^{(2)} \) ... Coordinates of the closest-point-projection of the slave particle onto the master surface at current configuration
Nonlinear Contact Kinematics

Normal Gap Function

\[ g_N \left( X^{(1)}, t \right) = - \left( \phi_t^{(1)} \left( X^{(1)} \right) - \phi_t^{(2)} \left( \bar{X}^{(2)} \left( X^{(1)}, t \right) \right) \right) \cdot \nu \]

\[ \nu = n^{(2)} \left( \bar{x}^{(2)} \left( \bar{X}^{(1)}, t \right), t \right) \]

\( g_N \quad \text{... Normal gap on current configuration} \)

\( g_N > 0 \quad \text{... Contact constraint is violated} \)

\( g_N \leq 0 \quad \text{... Contact constraint is satisfied} \)

\( \nu \quad \text{... Outward unit normal at the closest-point-projection on the master surface at current configuration} \)
Nominal Contact Traction, Nominal Contact Pressure

The nominal contact traction vector is defined as,

$$T^{(1)} \left( X^{(1)}, t \right) = P^{(1)} \left( X^{(1)}, t \right) \cdot N^{(1)} \left( X^{(1)} \right)$$

$$T^{(1)} \left( X^{(1)}, t \right) = -t_N \left( X^{(1)}, t \right) n^{(1)} \left( X^{(1)}, t \right)$$

where the nominal contact pressure is defined as,

$$t_N \left( X^{(1)}, t \right) = -T^{(1)} \left( X^{(1)}, t \right) \cdot n^{(1)} \left( X^{(1)}, t \right)$$

Setting $n^{(1)} \left( X^{(1)}, t \right) = -n^{(2)} \left( \bar{X}^{(2)} \left( X^{(1)}, t \right), t \right) = -\nu$

$$T^{(1)} \left( X^{(1)}, t \right) = t_N \left( X^{(1)}, t \right) \nu$$

$$t_N \left( X^{(1)}, t \right) = T^{(1)} \left( X^{(1)}, t \right) \cdot n^{(2)} \left( \bar{X}^{(2)} \left( X^{(1)}, t \right) \right) = T^{(1)} \left( X^{(1)}, t \right) \cdot \nu$$
Contact Kinematic/Pressure Constraints

Kühn-Tucker contact/separation optimality conditions

\[ t_N \left( X^{(1)}, t \right) \geq 0, \quad g_N \left( X^{(1)}, t \right) \leq 0, \quad t_N \left( X^{(1)}, t \right) g_N \left( X^{(1)}, t \right) = 0 \]

Contact consistency or persistency condition

If \[ g_N \left( X^{(1)}, t \right) = 0 \] then

\[ t_N \left( X^{(1)}, t \right) \geq 0, \quad \dot{g}_N \left( X^{(1)}, t \right) \leq 0, \quad t_N \left( X^{(1)}, t \right) \dot{g}_N \left( X^{(1)}, t \right) = 0 \]
Penalty Regularized Contact Constraints

The penalty regularization of the Kühn-Tucker contact/separation optimality conditions and contact persistency condition takes the form

\[ t_N (X^{(1)}, t) = \langle \varepsilon_N g_N (X^{(1)}, t) \rangle \]

where \( \varepsilon_N \) is the contact penalty parameter.

The penalty regularized contact constraints provides a constitutive-like equation for the nominal contact pressure as a function of the normal gap, allowing a displacement-driven formulation of the contact problem.
Augmented Lagrangian Regularized Contact Constraints

The augmented Lagrangian regularization of the Kühn-Tucker contact/separation optimality conditions and contact persistency condition take the form

\[ t_N \left( X^{(1)}, t \right) = \left\langle \lambda_N + \varepsilon_N g_N \left( X^{(1)}, t \right) \right\rangle \]

where \( \varepsilon_N \) is the contact penalty parameter and \( \lambda_N \) is the Lagrange multiplier subjected to the following Kühn-Tucker optimality constraints

\[ \lambda_N \geq 0, \quad g_N \leq 0, \quad \lambda_N g_N = 0 \]
Variational Contact Form

The contact variational contribution to the variational form of the momentum balance equation takes the form,

$$G_c \left( \varphi_t, \eta_0 \right) = \int_{\Gamma_c^{(1)}} t_N \delta g_N \, d\Gamma$$
Mechanical Contact Problem
Block-iterative Solution Scheme

Arrow-shape block system. Block-iterative solution scheme

Within the framework of penalty/augmented lagrangian methods, in order to get a better conditioned numerical problem, the resulting system of equations is arranged collecting cast, mould and interface variables, leading to a block arrow-shape system of equations of the form,

\[
\begin{bmatrix}
A_{\text{cast}} & 0 & A_{c,\text{cast}} \\
0 & A_{\text{mold}} & A_{c,\text{mold}} \\
A_{c,\text{cast}} & A_{c,\text{mold}} & A_c
\end{bmatrix}
\begin{bmatrix}
\Delta U_{\text{cast}} \\
\Delta U_{\text{mold}} \\
\Delta U_c
\end{bmatrix}
= -
\begin{bmatrix}
R_{\text{cast}} \\
R_{\text{mold}} \\
R_c
\end{bmatrix}
\]
Mechanical Contact Problem
Block-iterative Solution Scheme

Arrow-shape block system. Block-iterative solution scheme

The arrow-shape block system of equations can be solved using a block-iterative solution scheme given by,

\[
\begin{align*}
\mathbf{A}_{\text{cast}} \Delta \mathbf{U}^{(i+1)}_{\text{cast}} &= -\mathbf{R}_{\text{cast}} - \mathbf{A}_{c,\text{cast}} \Delta \mathbf{U}^{(i)}_{c} \\
\mathbf{A}_{\text{mold}} \Delta \mathbf{U}^{(i+1)}_{\text{mold}} &= -\mathbf{R}_{\text{mold}} - \mathbf{A}_{c,\text{mold}} \Delta \mathbf{U}^{(i)}_{c} \\
\mathbf{A}_{c} \Delta \mathbf{U}^{(i+1)}_{c} &= -\mathbf{R}_{c} - \mathbf{A}_{c,\text{cast}} \Delta \mathbf{U}^{(i+1)}_{\text{cast}} - \mathbf{A}_{c,\text{mold}} \Delta \mathbf{U}^{(i+1)}_{\text{mold}}
\end{align*}
\]
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Thermal Contact Problem

Heat Conduction

Heat conduction flux is given by,

\[ q_{\text{cond}} = h_{\text{cond}} (\Theta_c - \Theta_m) \]

where the heat conduction coefficient is considered to be a function of the contact pressure \( t_N \), thermal resistance by conduction \( R_{\text{cond}} \), Vickers hardness \( H_e \) and an exponent coefficient \( n \), and is given by,

\[ h_{\text{cond}} (t_N) = \frac{1}{R_{\text{cond}}} \left( \frac{t_N}{H_e} \right)^n \]
Thermal resistance by conduction $R_{\text{cond}}$ depends on the air trapped between cast and mould due to the surfaces roughness and on the mould coating, and is given by,

$$R_{\text{cond}} = \frac{R_z}{2k_a} + \frac{\delta_c}{k_c}$$

where $R_z$ is the mean peak-to-valley heights of rough surfaces, given by,

$$R_z = \sqrt{R_{z,\text{cast}}^2 + R_{z,\text{mould}}^2}$$

and $k_a$ is the thermal conductivity of the air trapped between the cast and mould surfaces roughness, $\delta_c$ is the coating thickness and $k_c$ is the thermal conductivity of the coating.
Heat convection flux is given by,

\[ q_{\text{conv}} = h_{\text{conv}} \left( \Theta_c - \Theta_m \right) \]

where the heat convection coefficient is considered to be a function of the contact gap \( g_N \), the mean peak-to-valley heights of rough surfaces \( R_z \), the thermal conductivity of the air trapped between the cast and mould surfaces roughness \( k_a \), the coating thickness \( \delta_c \) and the thermal conductivity of the coating \( k_c \), and is given by,

\[ h_{\text{conv}} (g_N) = \frac{1}{\max (g_N, R_z) / k_a + \delta_c / k_c} \]
Thermal Contact Problem

Heat Radiation

Heat radiation flux is given by,

\[ q_{rad} = \frac{\sigma_a \left( \Theta_c^4 - \Theta_m^4 \right)}{1/\varepsilon_c + 1/\varepsilon_m - 1} \]

where,

- \( \sigma_a \) … Boltzmann constant
- \( \Theta_c \) … cast temperature
- \( \Theta_m \) … mould temperature
- \( \varepsilon_c \) … cast emissivity
- \( \varepsilon_m \) … mould emissivity
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<th>Penalty</th>
<th>Augmented Lagrangian</th>
<th>Block-iterative Penalty</th>
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<tbody>
<tr>
<td>1</td>
<td>1.000000E+3</td>
<td>1.000000E+3</td>
</tr>
<tr>
<td>2</td>
<td>2.245836E+2</td>
<td>6.84654E+1</td>
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<tr>
<td>3</td>
<td>2.093789E+2</td>
<td>8.57626E-2</td>
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<tr>
<td>4</td>
<td>7.473996E+1</td>
<td>2.97468E+1</td>
</tr>
<tr>
<td>5</td>
<td>5.873453E+1</td>
<td>4.845342E-2</td>
</tr>
<tr>
<td>6</td>
<td>9.986438E+0</td>
<td>4.734127E-3</td>
</tr>
<tr>
<td>7</td>
<td>3.762686E-2</td>
<td>3.946447E-3</td>
</tr>
</tbody>
</table>
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Concluding Remarks

A suitable coupled thermomechanical model allowing the simulation of complex industrial casting processes has been introduced.

A thermomechanical J2 viscoplastic material model allowing a continuous transition from an initial liquid-like state to a final solid state has been introduced. The thermomechanical J2 viscoplastic model reduces to a purely deviatoric viscous model for the liquid-like phase.

An OSGS stabilized mixed formulation for tetrahedral elements has been used to avoid locking and spurious pressure oscillations due to the quasi-incompressibility constraints arising in J2 viscoplasticity models.

A thermomechanical contact model has been introduced. Ill conditioning induced by the penalty method used in the mechanical contact formulation has been smoothed introducing a block-iterative algorithm.

The formulation developed has been implemented in the FE software VULCAN and a number of computational simulations have been shown.