Modelling of heat transfer with phase transformation

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Casting process simulation

- Filling of the mold
- Solidification of the material
- Resolution of the heat equation with phase change (liquid → solid)

Modelling of heat transfer with phase transformation
Two difficulties for simulation:
1- material properties depends on temperature $T$
   - conductivity $k(T)$
   - mass density $\rho(T)$
   - heat capacity $c_p(T)$

2- Latent heat $L$ is released during solidification
   - heat source localized in the solidification range (called mushy zone for an alloy)
Thermal balance
\[ dH = \Phi \, dt \]

Enthalpy of the subdomain \( \omega(x) \) at time \( t \):
\[
H(\omega(x), t) = \int_{\omega(x)} \left( \int_{T_0}^{T(y, t)} \rho(\tau) c_p(\tau) \, d\tau \right) d\omega(y)
\]

Thermal flux from outside:
\[
\Phi(\omega(x), t) = \int_{\partial \omega(x)} k \nabla T \cdot n \, dS
\]

thanks to the divergence theorem:
\[
\Phi(\omega(x), t) = \int_{\omega(x)} \nabla \cdot (k \nabla T) \, d\omega(x)
\]
Enthalpy variation

\[ dH = H(\omega(x), t+dt) - H(\omega(x), t) = \int_{\omega(x)} \left( \int_{T(y,t)} \rho(\tau) c_p(\tau) d\tau \right) d\omega(y) \]

since

\[ T(y, t+dt) = T(y, t) + \frac{\partial T}{\partial t} dt + o(dt) \]

then

\[ \int_{T(y,t)} \rho(\tau) c_p(\tau) d\tau = \rho(T(y, t)) c_p(T(y, t)) \left( \frac{\partial T}{\partial t} dt + o(dt) \right) \]

and \( dH \) becomes

\[ dH = \left( \int_{\omega(x)} \rho(T(y, t)) c_p(T(y, t)) \frac{\partial T}{\partial t} d\omega(y) \right) dt + o(dt) \]
Finally, the thermal balance equation becomes

\[
\left( \int_{\omega(x)} \rho(T(y,t)) c_p(T(y,t)) \frac{\partial T}{\partial t} d\omega(y) \right) dt + o(dt) = \int_{\omega(x)} \nabla \cdot (k \nabla T) d\omega(x) dt
\]

if \( t \) vanishes, then

\[
\int_{\omega(x)} \rho(T(y,t)) c_p(T(y,t)) \frac{\partial T}{\partial t} d\omega(y) = \int_{\omega(x)} \nabla \cdot (k \nabla T) d\omega(x)
\]

and, because \( x \) and \( \omega(x) \) are arbitrary in \( \Omega \), we can write on any point \( x \) in \( \Omega \), the classical heat equation:

\[
\rho(T(x,t)) c_p(T(x,t)) \frac{\partial T}{\partial t} = \nabla \cdot (k(x,t) \nabla T(x,t))
\]
When solidification, enthalpy $H(T)$ becomes

$$H(\omega(x), t) = \int_{\omega(x)}^{T} \int_{t_0}^{T} \rho(\tau) c_p(\tau) d\tau d\omega(x)$$

for $T < T_{solidus}$

$$H(\omega(x), t) = \int_{\omega(x)}^{T_{solidus}} \int_{t_0}^{T_{solidus}} \rho(\tau) c_p(\tau) d\tau + \int_{T_{solidus}}^{T} \rho(\tau) c_p(\tau) d\tau + \rho(\tau) L_f (1 - f_s(\tau)) d\omega(x)$$

for $T_{solidus} < T < T_{liquidus}$

$$H(\omega(x), t) = \int_{\omega(x)}^{T_{solidus}} \int_{t_0}^{T_{solidus}} \rho(\tau) c_p(\tau) d\tau + \int_{T_{solidus}}^{T_{liquidus}} \rho(\tau) c_p(\tau) d\tau + \int_{T_{liquidus}}^{T} \rho(\tau) c_p(\tau) d\tau + \rho(\tau) L_f + \int_{T_{liquidus}}^{T} \rho(\tau) c_p(\tau) d\tau d\omega(x)$$

for $T > T_{liquidus}$

with $L_f$ latent heat

$f_s(T)$ solid fraction

Usual heat equation with solidification

$$\rho c_p(T) \frac{\partial T}{\partial t} = \text{div}(k(T) \text{grad}(T)) + \rho L_f \frac{\partial}{\partial t} [f_s(T)]$$

unstationnary  conduction  heat source (latent heat $L_f$)
Feulvarch (2009) proposed an alternative to the enthalpy method or source term method.

Heat equation written in enthalpy $H$:

$$\frac{\partial H}{\partial t} = \text{div} (k(T) \text{grad}(T))$$

$$T = g(H)$$
Feulvarch approach is more efficient than other ones to model heat latent release

How to solve this approach with Proper Generalized Decomposition (PGD)?
PGD principle:
the unknown is written in the form of separated variables

\[ T(x, t) = \sum_i \varphi_i(x) a_i(t) \]

PGD solves iteratively each \{\varphi_i(x), a_i(t)\} couple.

With Feulvarch approach: 2 unknowns and \( g(H) \) non linear

\[
\begin{align*}
\frac{\partial H}{\partial t} &= \text{div}(k \text{ grad}(T)) \\
T &= g(H)
\end{align*}
\]

Our choice: temperature is substituted, enthalpy becomes the only unknown

\[
\frac{\partial H}{\partial t} = \text{div}(k \text{ grad}(g(H)))
\]

\[ H(x, t) = \sum_i \varphi_i(x) a_i(t) \]
Studied 1D problem, in aluminum alloy:

\[
\begin{align*}
\frac{\partial H(x,t)}{\partial t} &= k \frac{\partial^2 g(H(x,t))}{\partial x^2} \\
\forall x &\in [0, L], \forall t \in [0, t_{\text{max}}] \\
T(x,0) &= 800 \, ^\circ C \\
H(x,0) &= g^{-1}(800) \\
T(0,t) &= 800 \left(1 - \frac{t}{t_{\text{max}}} \right) \\
H(0,t) &= g^{-1}(T(0,t)) \\
x = 0 \\
x = L
\end{align*}
\]
* Conductivity is a constant and uniform \( k = 100 \, W/K/m \)

* Function \( H = g^{-1}(T) \) is supposed to be continuous and bijective
Weak formulation

\[ \iint_{\Omega_x, \Omega_t} \frac{\partial H}{\partial t} T^* + \iint_{\Omega_x, \Omega_t} k \frac{\partial g(H)}{\partial x} \frac{\partial T^*}{\partial x} = 0 \quad \forall T^* \]

Finite element discretisation (space and time)

\[ H(x, t) = \sum_{i,j} N_i(x) H_{ij} P_j(t) = N^T(x) H P(t) \]

\[ g(H(x, t)) = g\left(\sum_{i,j} N_i(x) H_{ij} P_j(t)\right) = \sum_{i,j} N_i(x) g(H_{ij}) P_j(t) \]

\[ = N^T(x) G(H) P(t) \]

with \[ [G(H)]_{ij} = g(H_{ij}) \]
Discrete equation

\[ M H O + K G(H)Q = F \]

with

\[ M, K \] usual mass and stiffness matrices

\[ Q = \int_\Omega P^T(t)P(t)dt \quad O = \int_\Omega \frac{\partial P^T(t)}{\partial t}P(t)dt \]

Newton-Raphson iteration \( k \rightarrow k + 1 \)

\[
M[\delta H]O + K[G'(H^k) \circ \delta H]Q = R(H^k) \tag{1}
\]

\[ H^{k+1} = [\delta H] + H^k \]

with \[ [G'(H)]_{ij} = g'(H_{ij}) \]
PGD resolution

Greedy algorithm:

Enrichment iteration \( j \rightarrow j+1 \)

\[
[\delta H]^{j+1} = [\delta H]^j + [r s^T]
\]

Fixed alternating iterations:

(1) projected on \( s \)

\[
A_1 r = b_1 \rightarrow r
\]

(1) projected on \( r \)

\[
A_2 s = b_2 \rightarrow s
\]
Algorithm

Newton-Raphson $k$

Enrichment $j$

Fixed point

$A_1 r = b_1$

$A_2 s = b_2$

$[\delta H]^{j+1} = [\delta H] + [r s^T]$

$H^{k+1} = [\delta H] + H^k$
Latent heat release through $T = g(H)$

As described, PGD algorithm does not converge!
We have to introduce the latent heat progressively (6 steps)

![Graph showing latent heat progression]

Latent heat iterations
- Newton-Raphson
- Enrichment
- Fixed point

\[
\begin{align*}
\delta H_{j+1} &= \delta H_j + r \cdot s^T \\
H_{k+1} &= H_k + \delta H_{j+1}
\end{align*}
\]

Modelling of heat transfer with phase transformation
Studied 1D problem, in aluminum alloy:

\[ x = 0, \quad x = 0.1L, \quad x = L \]

\[ \text{Relative error} \quad e = \max_t \frac{\| T_{\text{imp}}(t) - T_{\text{PGD}}(t) \|}{\| T_{\text{imp}}(t) \|} = 0.5\% \]

100 elements on space
40 elements on time

Modelling of heat transfer with phase transformation
Conclusion

- PGD used to simulate solidification process
- original formulation of the solidification
- error was excellent

Perspectives

- 2D and 3D problem
- conductivity depends on $T$
- more exact $H(T)$ function

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