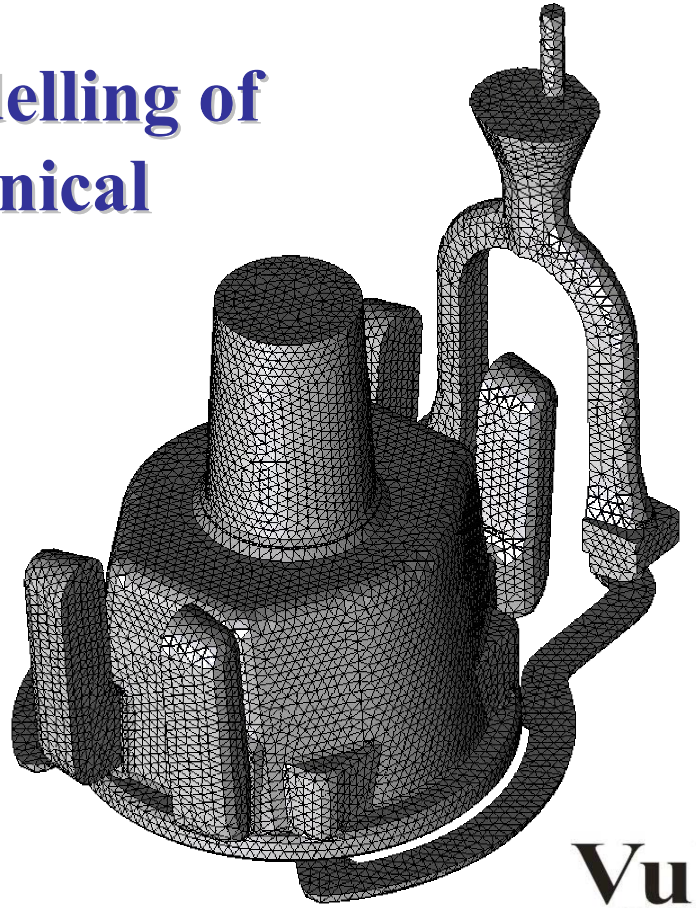
On the Constitutive Modelling of Coupled Thermo-Mechanical Phase-Chang Problems



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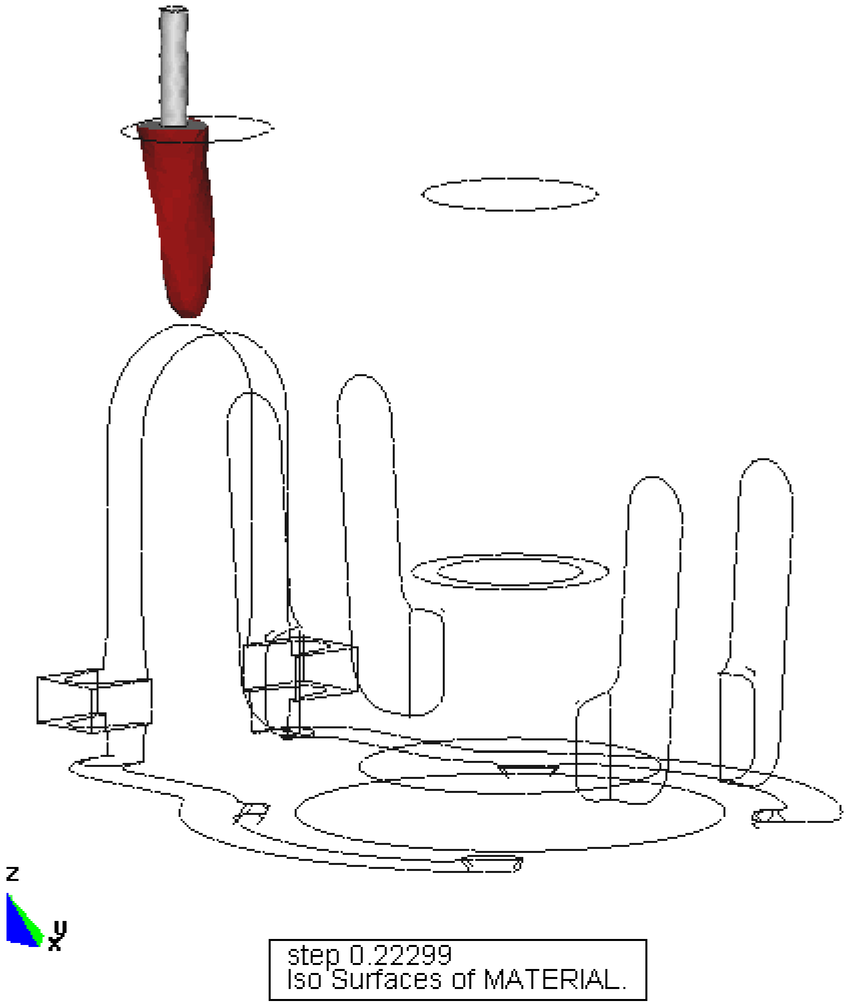
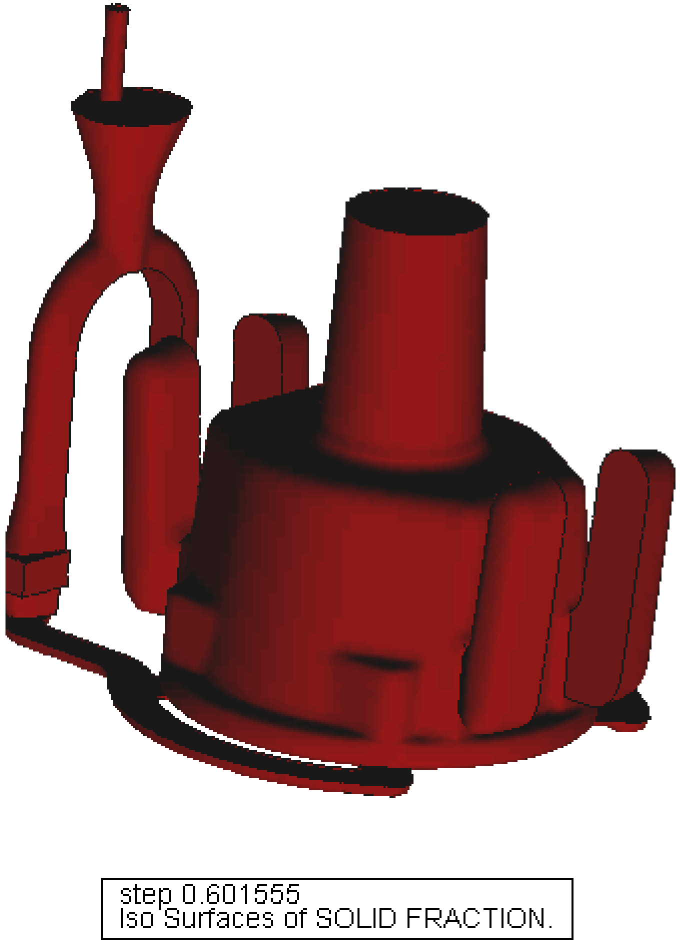
Problematic in a Casting Simulation

- **Accurate simulation** of the thermo-mechanical behaviour is crucial to achieve a truthful casting simulation especially for aluminium alloys in permanent moulds.
- **Material behaviour** strongly depends on temperature. Liquid, semi-solid and solid phases must be considered.
- **Contact interaction** among all casting tools is a consequence of the thermal deformations generated by high temperature gradients and phase transformations during solidification and cooling processes.
- Really complex geometries are discretized using tetrahedral meshes. Standard Galerkin formulation is not suitable for such a problem especially if **incompressible behaviour** occurs.

Casting Simulation: Filling and Solidification

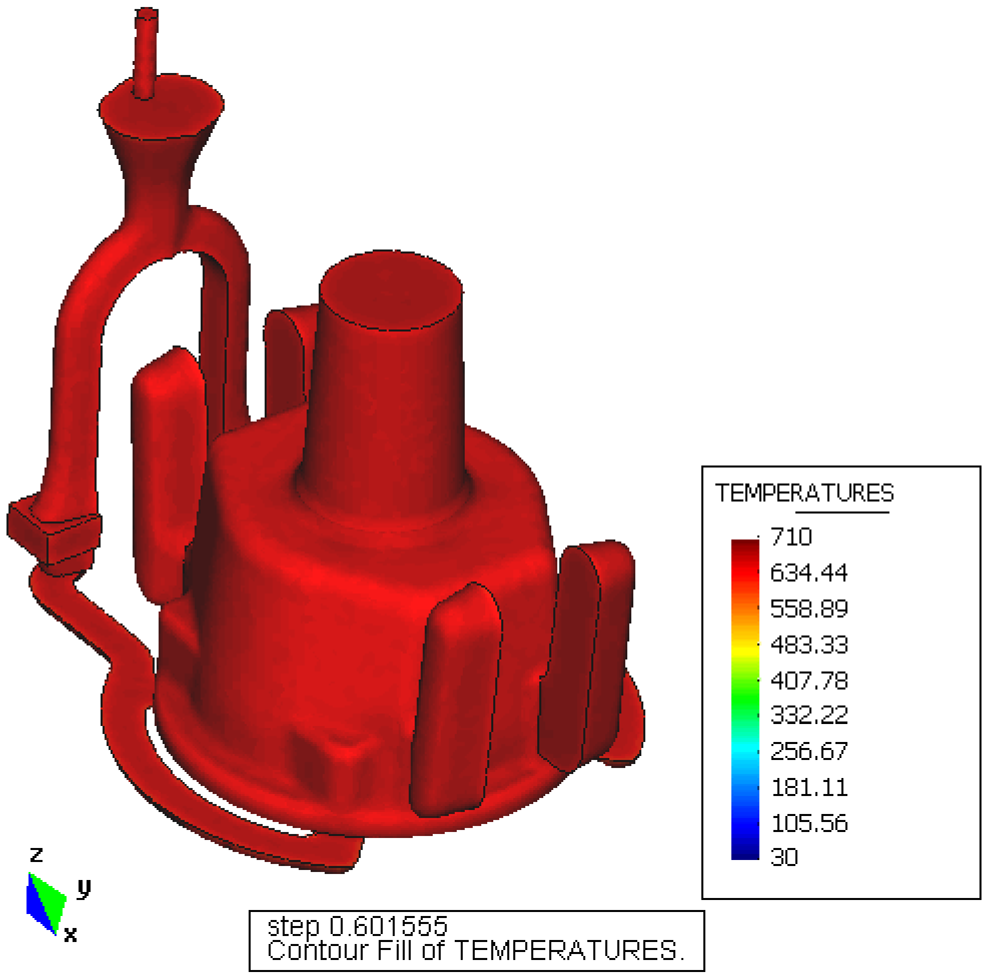


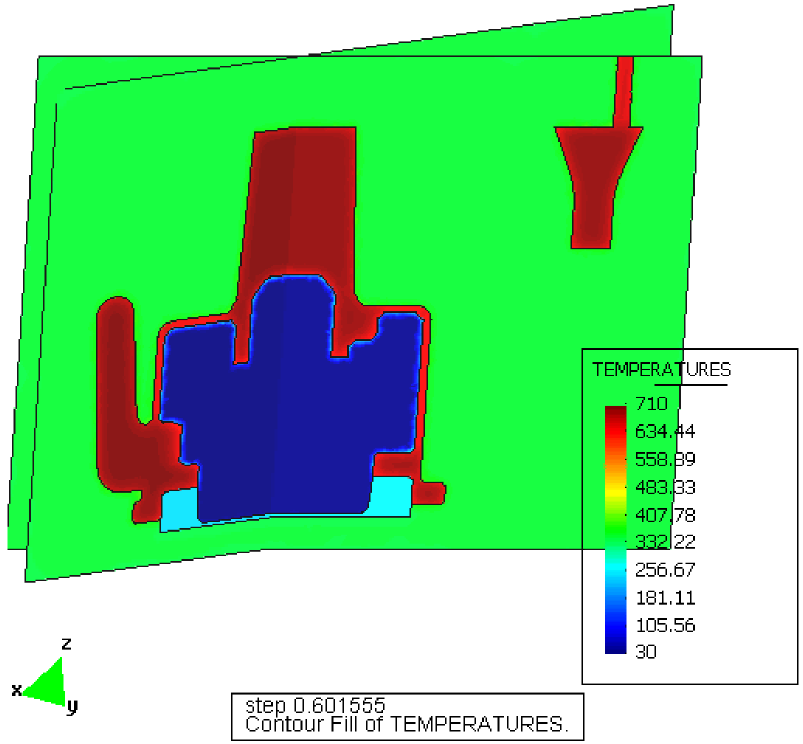
Filling Analysis



Solidification Analysis

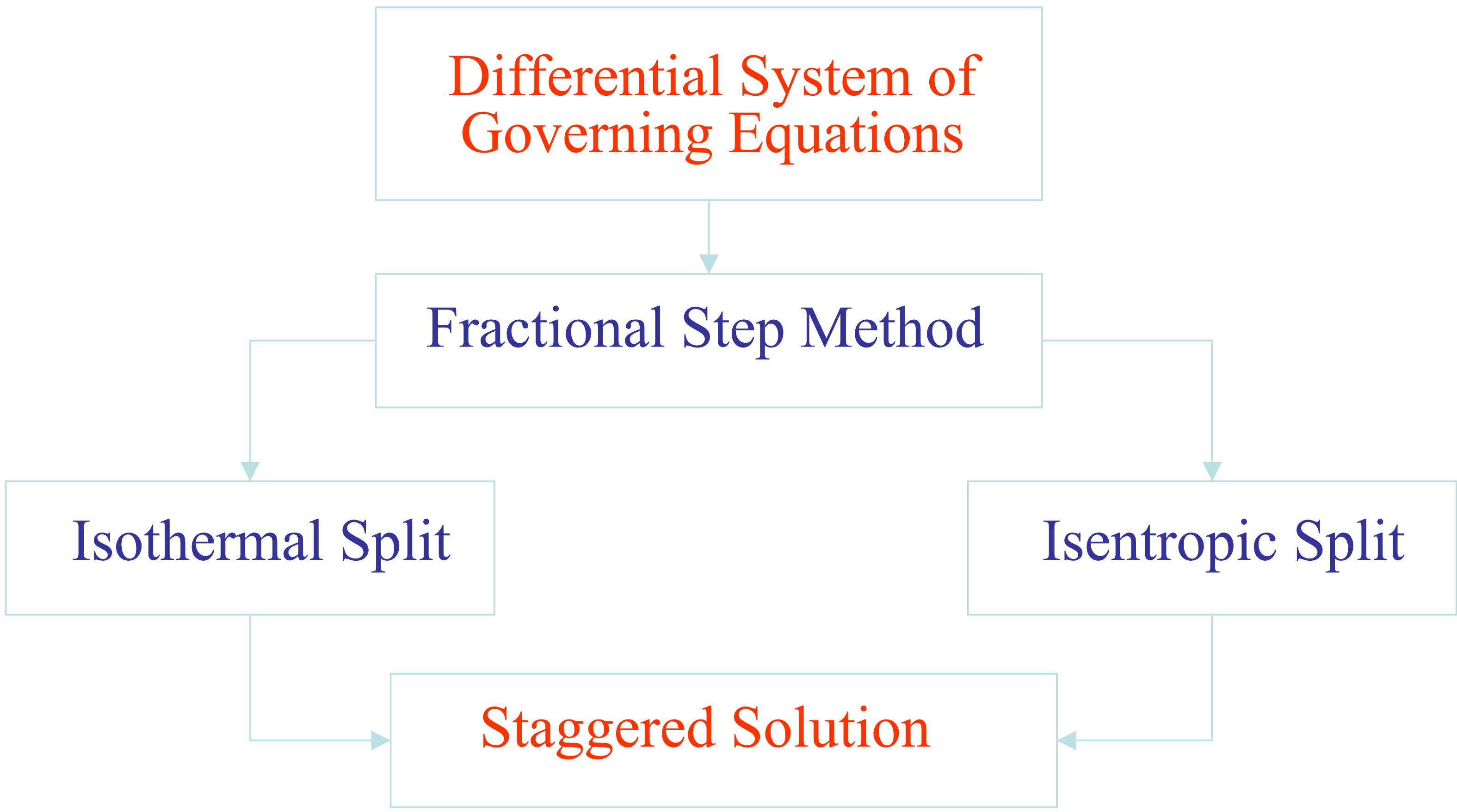
Casting Simulation: Cooling





Cooling Analysis

Casting Simulation: Coupling Strategy



Coupled Thermo-Mechanical Problem

Balance of Energy Equation

$$\left\langle C\dot{\Theta} + \dot{L}, \delta\vartheta \right\rangle + \left\langle k\,\nabla\Theta, \nabla\,\delta\vartheta \right\rangle = -\left\langle \bar{q}, \delta\vartheta \right\rangle_{\partial\Omega} - \left\langle q_c, \delta\vartheta \right\rangle_{\partial\Omega c}$$

Fractional step method
Staggered product formula solution algorithm

LOOP, TIME

– Solve Thermal problem at constant configuration

⇨ Temperature

– Solve Mechanical problem at constant temperature

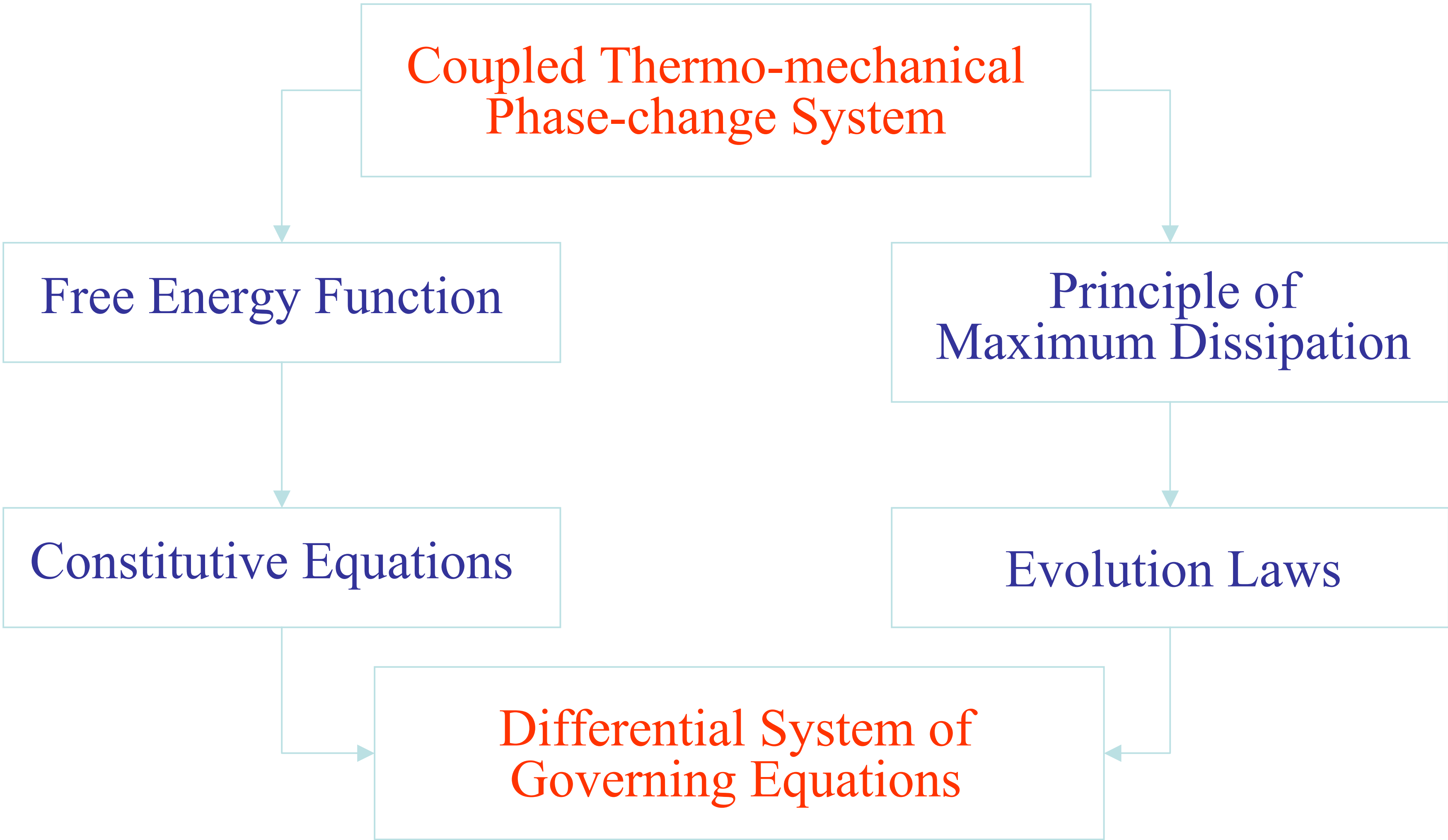
⇨ Displacements, Stresses

END-LOOP

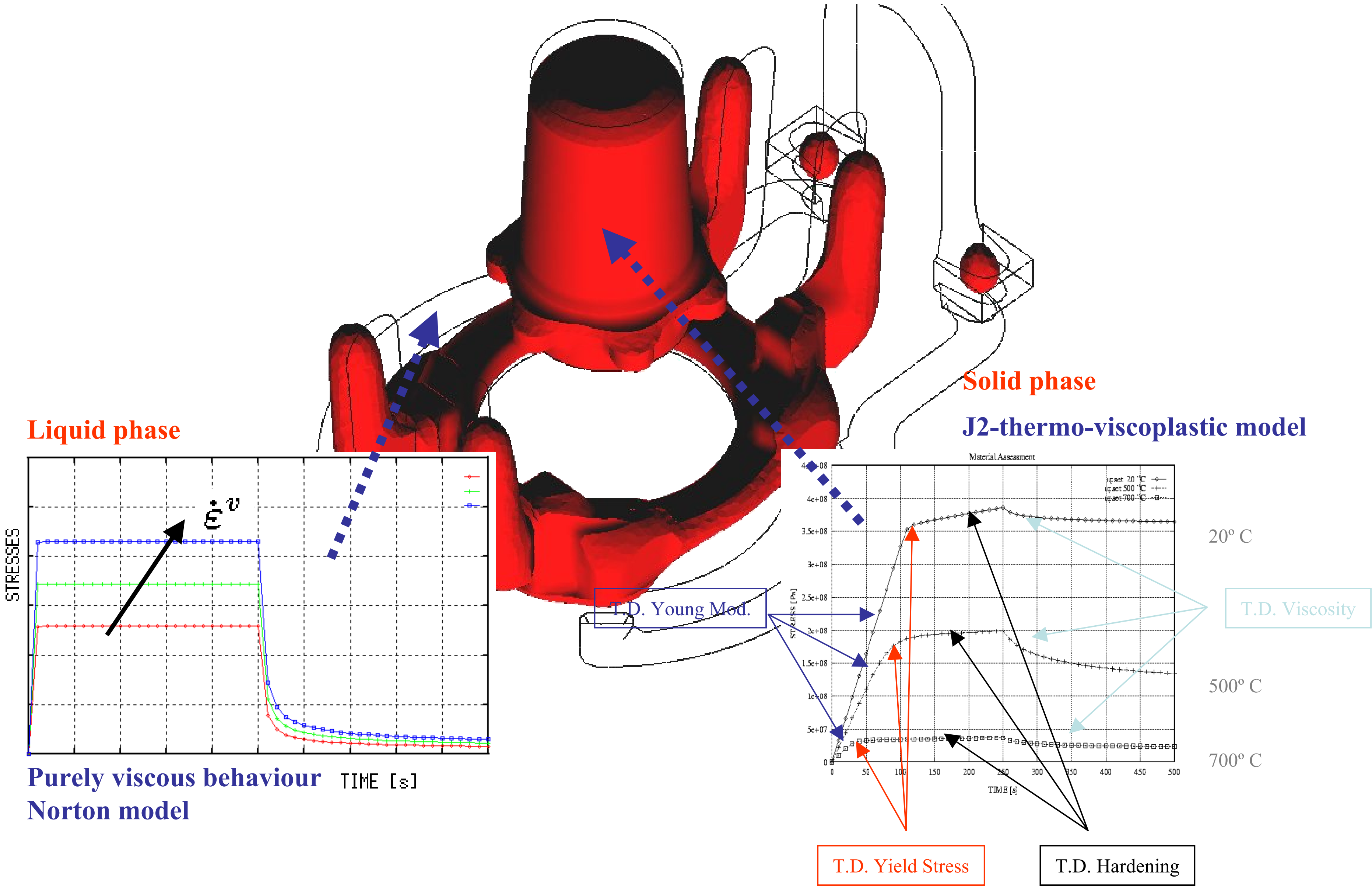
Balance of Momentum Equation

$$\left\langle \nabla^s \delta\mathbf{v}, \sigma \right\rangle = \left\langle \delta\mathbf{v}, \mathbf{b} \right\rangle + \left\langle \delta\mathbf{v}, \bar{\mathbf{t}} \right\rangle_{\partial\Omega} + \left\langle \delta\mathbf{v}, \mathbf{t}_c \right\rangle_{\partial\Omega c}$$

Casting Simulation: Theoretical Framework



Mechanical Behaviour



Mechanical Evolution laws

- Additive decomposition of the inelastic strain tensor

$$\dot{\varepsilon}^{I} = \dot{\varepsilon}^{v} + \dot{\varepsilon}^{vp}$$

- J2-Visco-plastic evolution laws (solid phase)

$$\Phi(\mathbf{s}, \mathbf{q}, q, \Theta) = \|\mathbf{s} - \mathbf{q}\| - R(q, \Theta) \leq 0$$

$$R(q, \Theta) = \sqrt{\frac{2}{3}}\left[\sigma_0(\Theta) - q\right]$$

$$\begin{cases} \gamma^{vp} = \dfrac{1}{\eta^{vp}} \langle \Phi(\boldsymbol{\Sigma}, \Theta) \rangle^{n} \\ \mathbf{n} = \dfrac{\mathbf{s} - \mathbf{q}}{\|\mathbf{s} - \mathbf{q}\|} = \dfrac{\boldsymbol{\beta}}{\|\boldsymbol{\beta}\|} \end{cases}$$

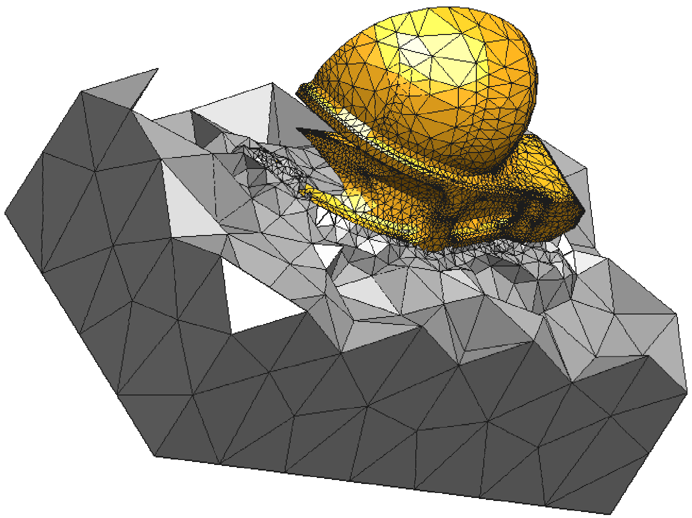
$$\begin{aligned} \dot{\varepsilon}^{p} &= \gamma^{vp} \frac{\partial \Phi(\mathbf{s}, \mathbf{q}, q, \Theta)}{\partial \mathbf{s}} = \gamma^{vp}\,\mathbf{n} \\ \dot{\zeta} &= \gamma^{vp} \frac{\partial \Phi(\mathbf{s}, \mathbf{q}, q, \Theta)}{\partial \mathbf{q}} = -\gamma^{vp}\,\mathbf{n} \\ \dot{\xi} &= \gamma^{vp} \frac{\partial \Phi(\mathbf{s}, \mathbf{q}, q, \Theta)}{\partial q} = \gamma^{vp} \sqrt{\frac{2}{3}} \end{aligned}$$

- Purely viscous strains (liquid-like phase)

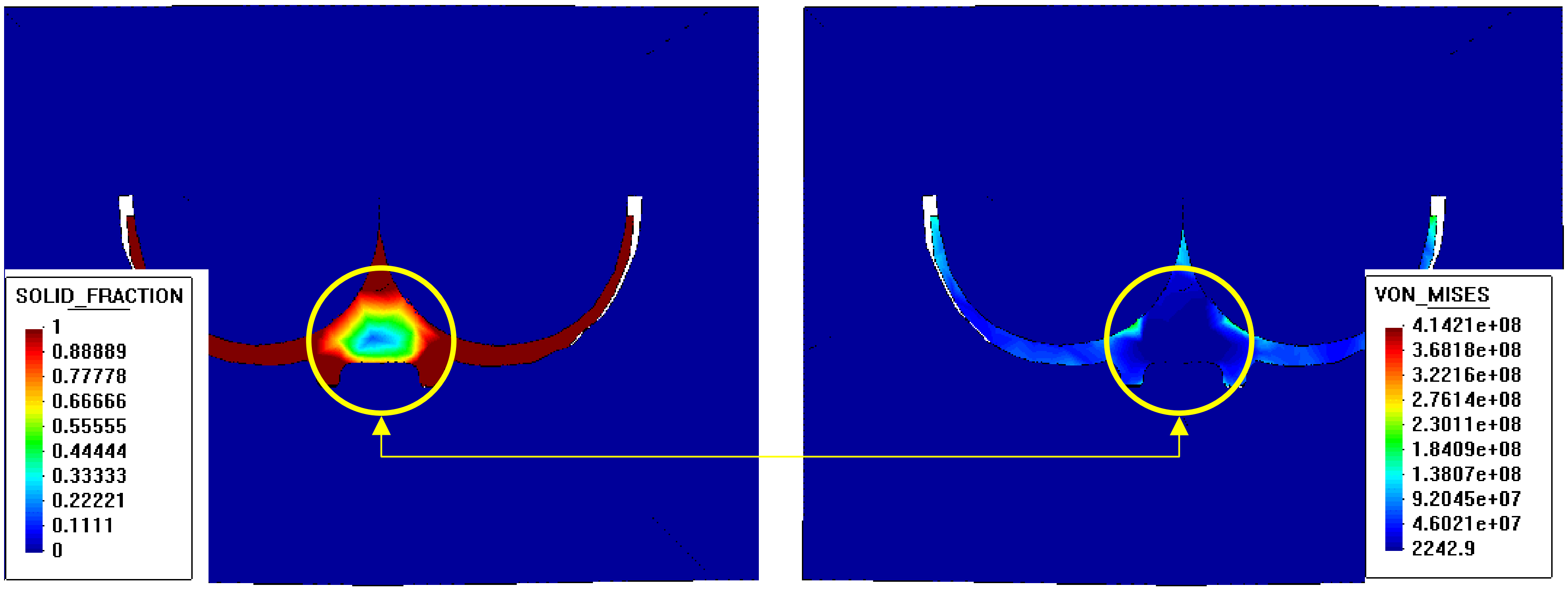
Particular case of the previous model when no hardening is considered and von-Mises radio tents to zero $R(\Theta) \rightarrow 0$

$$\dot{\varepsilon}^{v} = \frac{1}{\eta^{v}} \mathbf{s}$$

Mechanical Behaviour



When the material is still liquid
no deviatoric stresses are generated



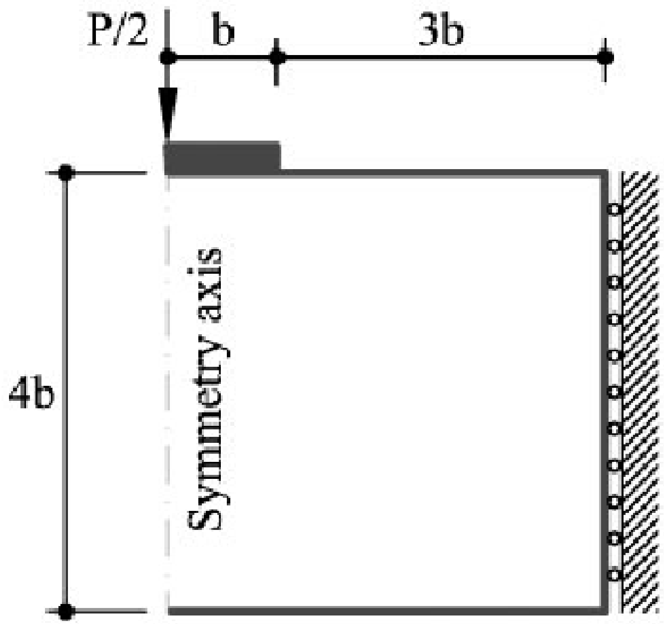
Mechanical Behaviour

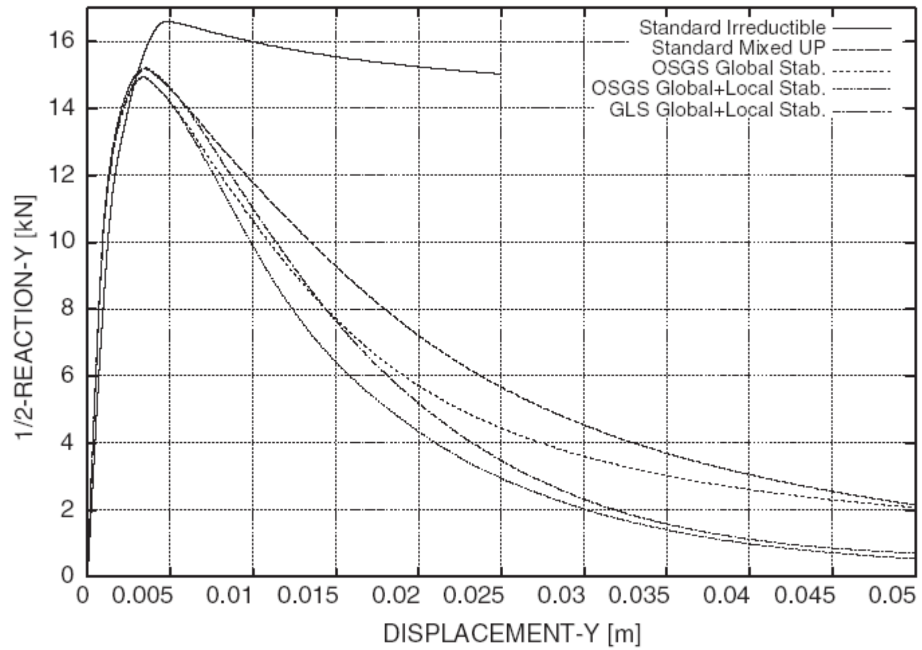
- Liquid phase:
  - Liquid-like behaviour
  - Purely viscous model
  - No thermal deformation

- Solid phase:
  - Solid-like behaviour
  - Thermal J2-viscoplasticity (plastic deformation is deviatoric)

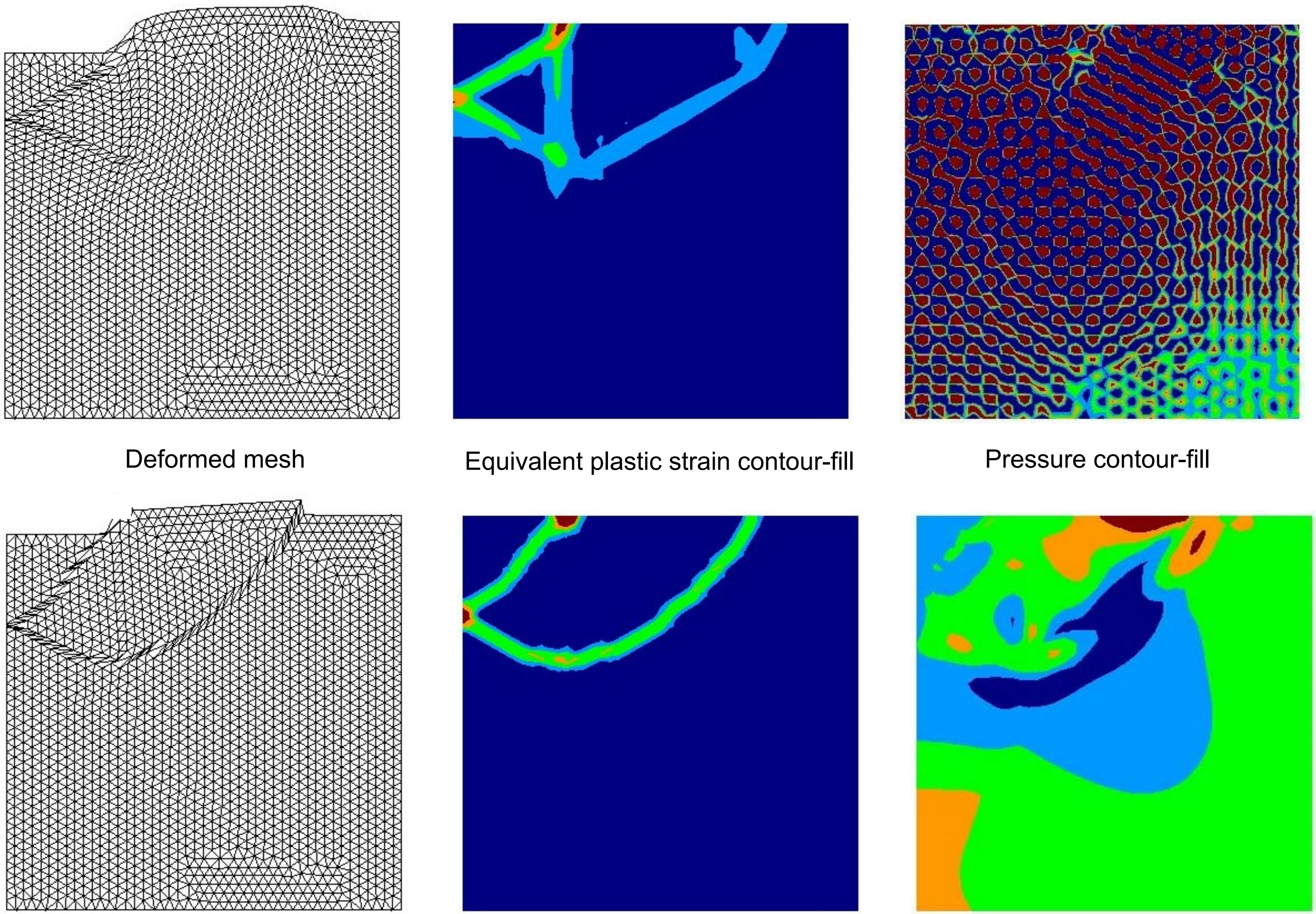
Incompressibility behaviour

Mechanical Mixed Formulation





Standard irreducible formulation



Mixed u/p formulation: OSGS Stabilization

Mechanical Mixed Formulation

- Mixed u/p formulation to deal with incompressibility

$$\begin{cases} \nabla\cdot\mathbf{s}+\nabla p+\mathbf{f} = \mathbf{0} & \text{in } \Omega \\ \nabla\cdot\mathbf{u}-\frac{1}{K}p = 0 & \text{in } \Omega \\ \mathbf{u} = \mathbf{0} & \text{on } \partial\Omega_u \\ \boldsymbol{\sigma}\cdot\mathbf{n} = \bar{\mathbf{t}} & \text{on } \partial\Omega_t \end{cases}$$

$$\boldsymbol{\sigma}(p,\mathbf{u}) = p\,\mathbf{1} + \mathbf{s}(\mathbf{u}) \qquad \begin{cases} p = \frac{1}{3}\operatorname{tr}(\boldsymbol{\sigma}) \\ \mathbf{s} = \operatorname{dev}(\boldsymbol{\sigma}) \end{cases}$$

$$K\to\infty \qquad \nabla\cdot\mathbf{u}=0 \qquad \text{in } \Omega$$

- Sub-grid scale method (Hughes-1995)

$$\mathcal{W} = \mathcal{W}_h \oplus \widetilde{\mathcal{W}} \longrightarrow \boxed{\mathbf{U} = \mathbf{U}_h + \widetilde{\mathbf{U}}} \qquad \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{u}_h \\ p_h \end{bmatrix} + \begin{bmatrix} \tilde{\mathbf{u}} \\ 0 \end{bmatrix}$$

$$R(\mathbf{U},\mathbf{V}_h) = R(\mathbf{U}_h,\mathbf{V}_h) + R\left(\widetilde{\mathbf{U}},\mathbf{V}_h\right) = \mathbf{0} \qquad \forall \mathbf{V}_h \in \mathcal{W}_{h,0}$$

- Orthogonal sub-grid scale method (Codina-2000)

$$\boxed{\widetilde{\mathcal{W}} \approx \mathcal{W}_h^{\perp}} \longrightarrow \widetilde{\mathbf{U}} \approx \tau\,\left[\nabla p_h - P_h(\nabla p_h)\right] \in \mathcal{W}_h^{\perp} \qquad \tau = c\left(\frac{2\mu}{h^2}\right)^{-1}$$

Mechanical Mixed Formulation

- Weak form: orthogonal sub-grid scale method (Chiumenti *et al.* 2002)

$$\begin{cases} \langle \nabla^s \mathbf{v}_h, \mathbf{s}_h \rangle + \langle \nabla \cdot \mathbf{v}_h, p_h \rangle - \langle \mathbf{v}_h, \mathbf{f} \rangle - \langle \mathbf{v}_h, \bar{\mathbf{t}} \rangle_{\partial\Omega} = 0 \\ \langle q_h, \nabla \cdot \mathbf{u}_h \rangle - \left\langle q_h, \frac{1}{K} p_h \right\rangle - \sum_{e=1}^{n_{elm}} \tau_e \, \langle \nabla q_h \cdot [\nabla p_h - \mathbf{\Pi}_h] \rangle = 0 \\ \langle \nabla p_h \, , \, \boldsymbol{\eta}_h \rangle - \langle \mathbf{\Pi}_h, \, \boldsymbol{\eta}_h \rangle = 0 \end{cases}$$

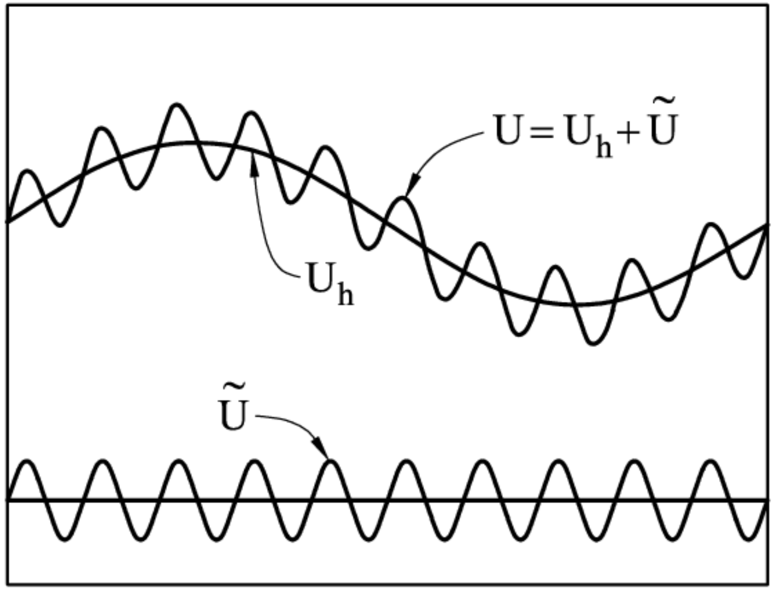
- Solution algorithm

Algorithm to solve the stabilized system
Solve at global level $\mathbf{U}^{(i)}$ and $\mathbf{P}^{(i)}$: $\begin{bmatrix} \mathbf{K}_{dev} & \mathbf{G} \\ \mathbf{G}^T & -\frac{1}{K}\mathbf{M}_p - \tau\,\mathbf{L} \end{bmatrix} \begin{bmatrix} \mathbf{U}^{(i)} \\ \mathbf{P}^{(i)} \end{bmatrix} = \begin{bmatrix} \mathbf{F} \\ -\tau\,\mathbf{G}^T \cdot \mathbf{\Pi}^{(i-1)} \end{bmatrix}$ Compute and store: $\mathbf{\Pi}^{(i)} = \mathbf{M}^{-1} \left(\mathbf{G}\mathbf{P}^{(i)} \right)$ Perform next iteration: i $\leftarrow i + 1$

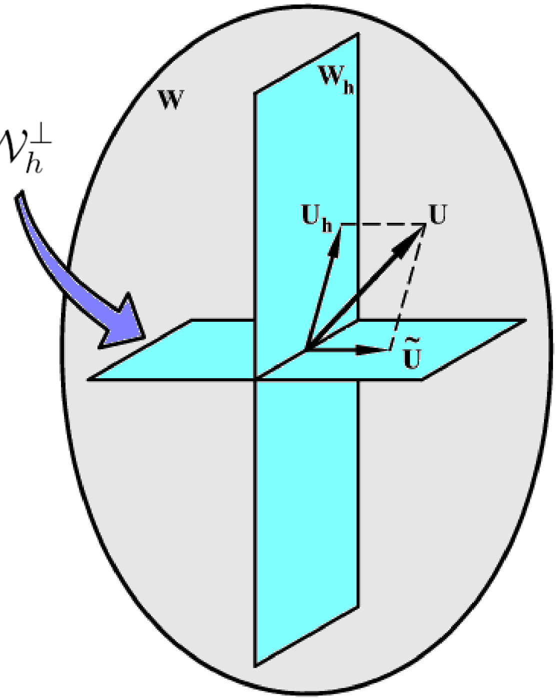
Mechanical Mixed Formulation

The exact solution includes components that cannot be captured within the Finite Element space

→ The method considers the effect of the Sub-Scale: enhanced solution



$\widetilde{\mathcal{W}} \approx \mathcal{W}_h^{\perp}$



The natural space to seek for the sub-scales is the orthogonal space to the FE approximation space

$$\tilde{\mathbf{U}} = \boldsymbol{\tau}_e P_h^{\perp}\left\{\mathcal{R}_h\right\}$$

Thermal Formulation

- Weak form of the balance of energy equation: enthalpy formulation

$$\left\langle \dot{H}, \delta\vartheta \right\rangle + \left\langle k\,\nabla\Theta, \nabla\,\delta\vartheta \right\rangle = \left\langle R + D_{mech} - H^{ep}, \delta\vartheta \right\rangle - \left\langle \bar{q}, \delta\vartheta \right\rangle_{\partial\Omega} - \left\langle q_c, \delta\vartheta \right\rangle_{\partial\Omega c}$$

- Enthalpy rate

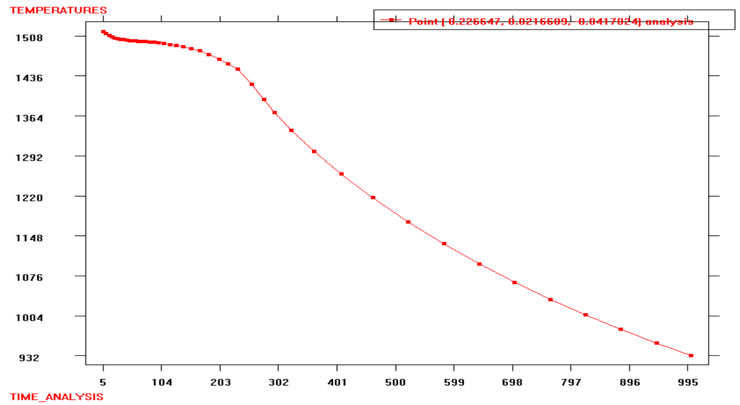
$$\dot{H}(\Theta) = C\dot{\Theta} + \dot{L}(\Theta)$$

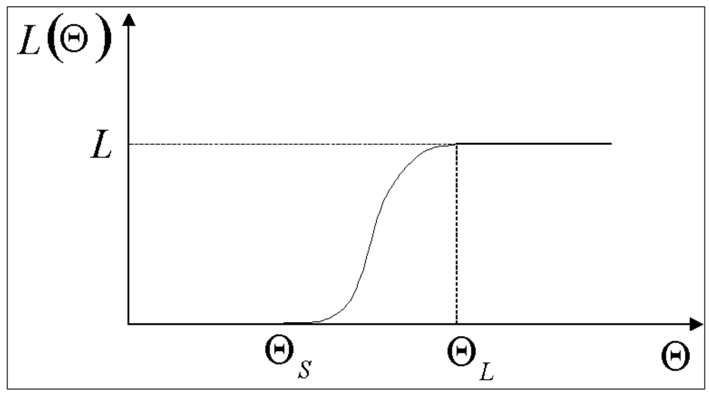
- Latent heat release

$$\dot{L}(\Theta) = L\,\frac{df_S(\Theta)}{d\Theta}\,\dot{\Theta}$$

- Solid fraction function

$$f_S(\Theta) = \begin{cases} 0 & if \quad \Theta > \Theta_L \\ f_S(\Theta) & if \quad \Theta_S \le \Theta \le \Theta_L \\ 1 & if \quad \Theta < \Theta_S \end{cases}$$





Mechanical Contact

- Penalty method: slave-master contact surfaces interaction

  - Definition of the mechanical gap:

$$g_n = \mathbf{n}^t \cdot \left[\left(\mathbf{X}^{(s)} + \mathbf{u}^{(s)} \right) - \left(\mathbf{X}^{(m)} + \mathbf{u}^{(m)} \right) \right] = u_n^{(s)} - u_n^{(m)}$$

  - Contact pressure: penalty parameter

$$t_c = \left\langle k\, g_n \right\rangle$$

$$\begin{cases} t_c \geq 0 & if \quad g_n = 0 \\ t_c = 0 & if \quad g_n \geq 0 \end{cases}$$

- Augmented lagrangian method

  - Contact pressure: augmented lagrangian regularization

$$t_c = \left\langle \lambda^i + k\, g_n \right\rangle$$

  - Lagrange multipliers:

$$\lambda^{i+1} = \lambda^i + t_c$$

Mechanical Contact

- Block-iterative solution & penalty method (Chiumenti *to appear*)
  - Decomposition of the final system of equation into casting, mould and coupled-contact equations: **arrow-shaped** system of equations

$$\begin{bmatrix} \mathbf{A}_{cast} & \mathbf{0} & \mathbf{A}_{c,cast} \\ \mathbf{0} & \mathbf{A}_{mold} & \mathbf{A}_{c,mold} \\ \mathbf{A}_{c,cast} & \mathbf{A}_{c,mold} & \mathbf{A}_{c} \end{bmatrix} \begin{Bmatrix} d\mathbf{u}_{cast} \\ d\mathbf{u}_{mold} \\ d\mathbf{u}_{c} \end{Bmatrix} = \begin{Bmatrix} \mathbf{r}_{cast} \\ \mathbf{r}_{mold} \\ \mathbf{r}_{c} \end{Bmatrix}$$

  - Block-iterative solution:

$$\begin{cases} \mathbf{A}_{cast}\, d\mathbf{u}_{cast}^{i+1} = \mathbf{r}_{cast} - \mathbf{A}_{c,cast}\, d\mathbf{u}_{c}^{i} \\ \mathbf{A}_{mold}\, d\mathbf{u}_{mold}^{i+1} = \mathbf{r}_{mold} - \mathbf{A}_{c,mold}\, d\mathbf{u}_{c}^{i} \\ \mathbf{A}_{c}\, d\mathbf{u}_{c}^{i+1} = \mathbf{r}_{c} - \mathbf{A}_{c,cast}\, d\mathbf{u}_{cast}^{i+1} - \mathbf{A}_{c,mold}\, d\mathbf{u}_{mold}^{i+1} \end{cases}$$

Thermal Contact

- Heat radiation

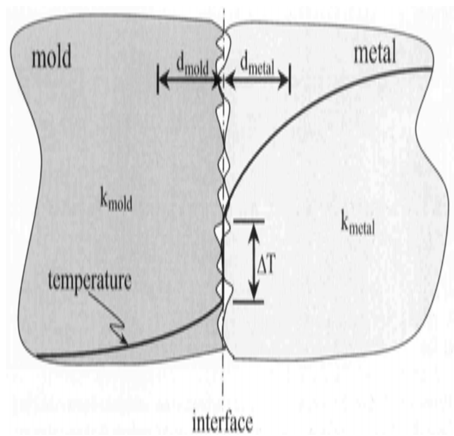
$$q_{rad} = \frac{\sigma_a\left(\Theta_c^4 - \Theta_m^4\right)}{\left(1/\varepsilon_c + 1/\varepsilon_m - 1\right)}$$

- Heat conduction

$$q_{cond} = h_{cond}\left(\Theta_c - \Theta_m\right)$$

$$h_{cond}\left(t_N\right) = \frac{1}{R_{cond}}\left(\frac{t_N}{H_e}\right)^n$$

$$\begin{cases} R_{cond} = 0.5\dfrac{R_z}{k_a} + \dfrac{\delta_c}{k_c} \\ R_z = \sqrt{R_{z,cast}^2 + R_{z,mold}^2} \end{cases}$$



- Heat convection

$$q_{conv} = h_{conv}\left(\Theta_c - \Theta_m\right)$$

$$h_{conv}\left(g_N\right) = \frac{1}{\max\left(g_N, R_z\right)/k_a + \delta_c/k_c}$$

Coupled Thermo-Mechanical Contact

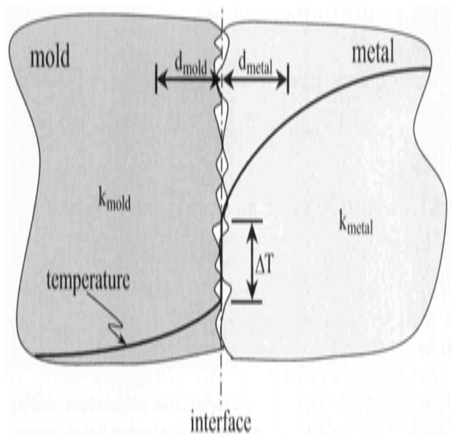
Mechanical **gap** induced by thermal contraction

Mechanical Contact

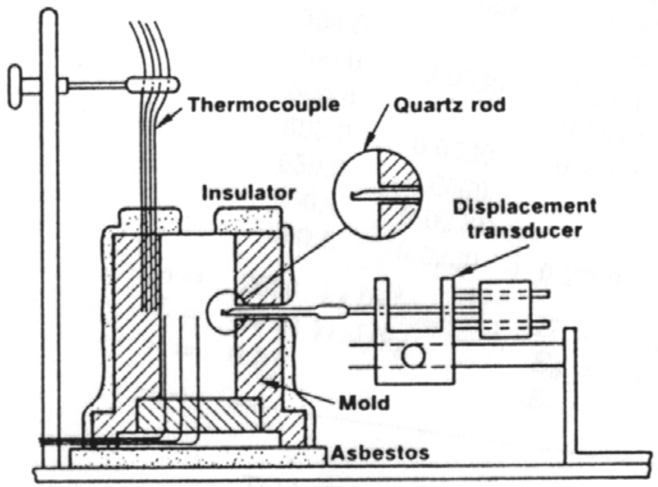
Thermal Contact: heat conduction & convection

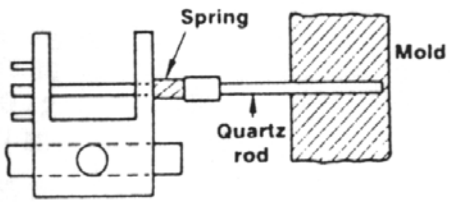
$$\begin{cases} Q^{(i)}_{c,\,cond} = h^{(i)}_{cond}\,(t_N, \Theta_g)\; g^{(i)}_{\Theta} \\ g^{(i)}_{\Theta} = \left(\Theta^{(i)} - \Theta_c\right) \\ h_{cond}\,(t_N) = h_{co}\left(\dfrac{t_N}{H_e}\right)^{\epsilon} \end{cases}$$

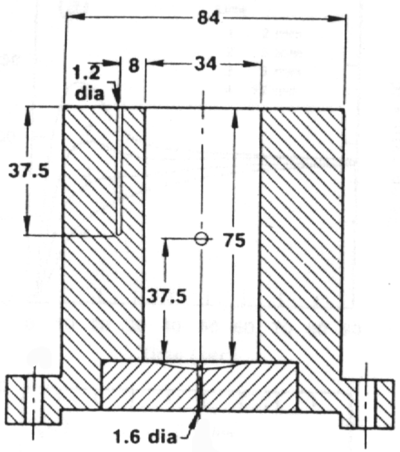
$$\begin{cases} Q^{(i)}_{c,\,conv} = h^{(i)}_{conv}\,(g_N)\; \bar{g}^{(i)}_{\Theta} \\ \bar{g}^{(i)}_{\Theta} = \left(\Theta^{(i)} - \Theta_g\right) \\ h_{conv}\,(g_N) = \dfrac{k_a}{g_N + \dfrac{k_a}{h_{o,\,conv}}} \end{cases}$$

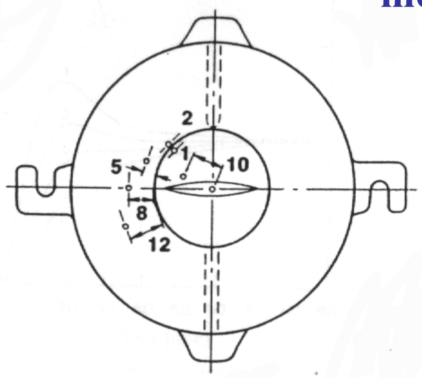


Analysis Optimization by Inverse Analysis



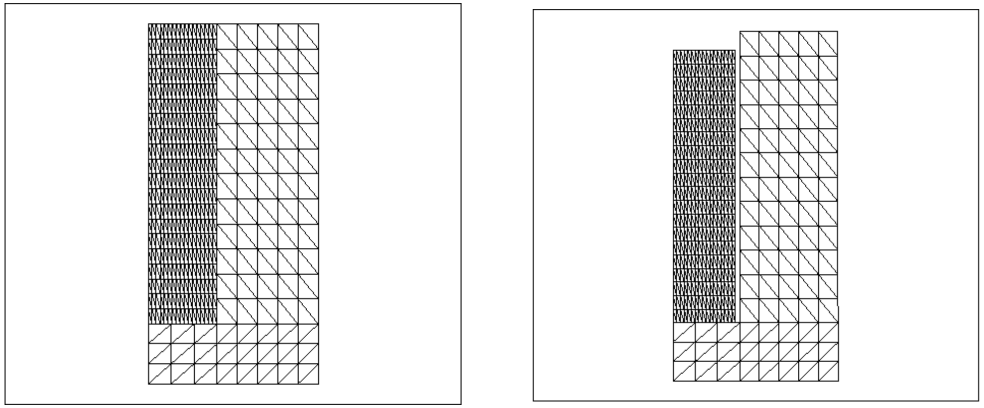




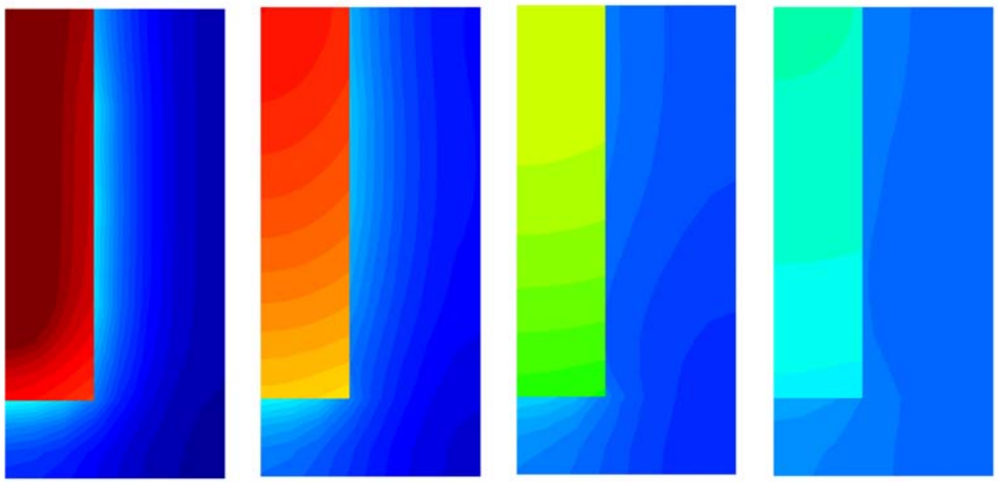


Experimental setup to get **temperature** evolution during solidification and cooling phases as well as the **mechanical gap** formation.

Analysis Optimization by Inverse Analysis



Original and deformed meshes



Temperature evolution during solidification and cooling processes

Numerical simulation of both solidification and cooling processes

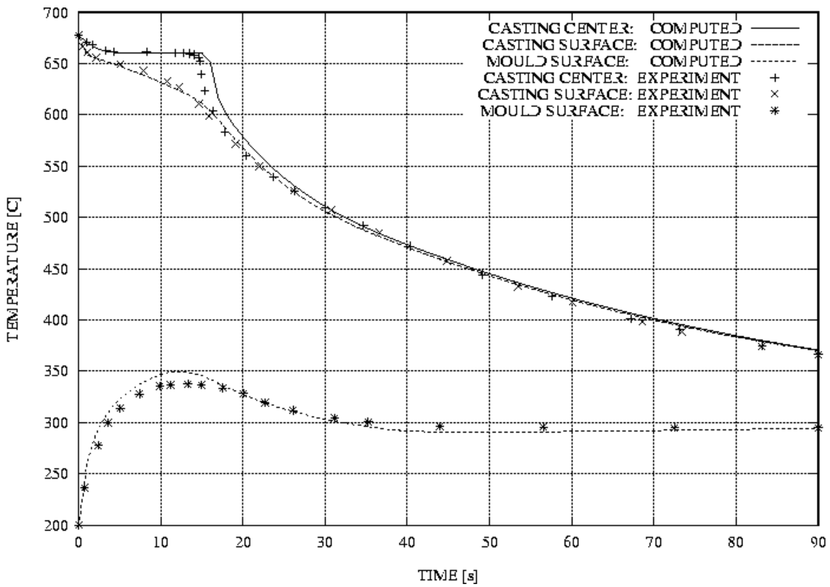
Analysis Optimization by Inverse Analysis

- An extra loop is added to the simulation system to add an optimization procedure based on **neuronal network** and **genetic algorithms**.

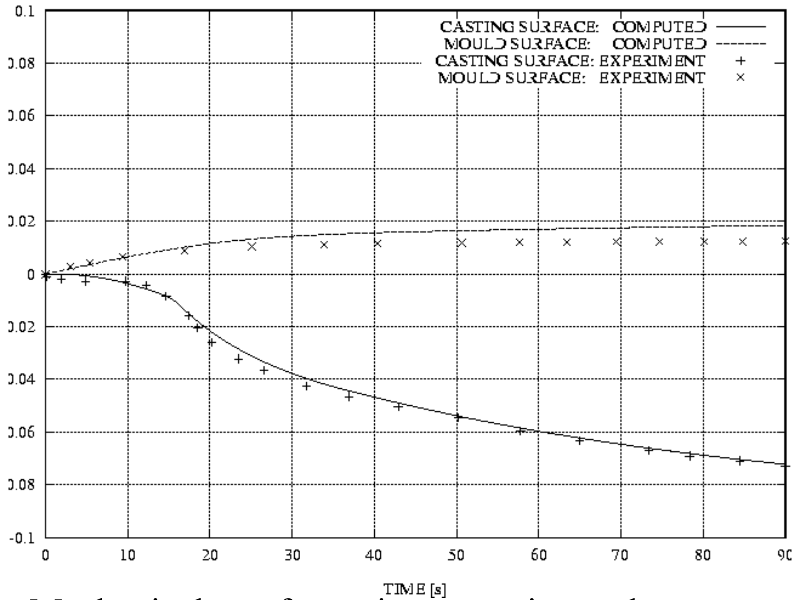
- **Inverse analysis algorithm** is considered to enhance the software response in term of results accuracy.

- Experimental results of benchmark test cases are reproduced in term of thermal and mechanical response **optimising the thermo-mechanical material data-base**.

Analysis Optimization by Inverse Analysis



Temperature evolution during solidification and cooling processes at the casting center, casting surface and mold surface: experimental vs. computed values.



Mechanical gap formation: experimental vs. computed values.

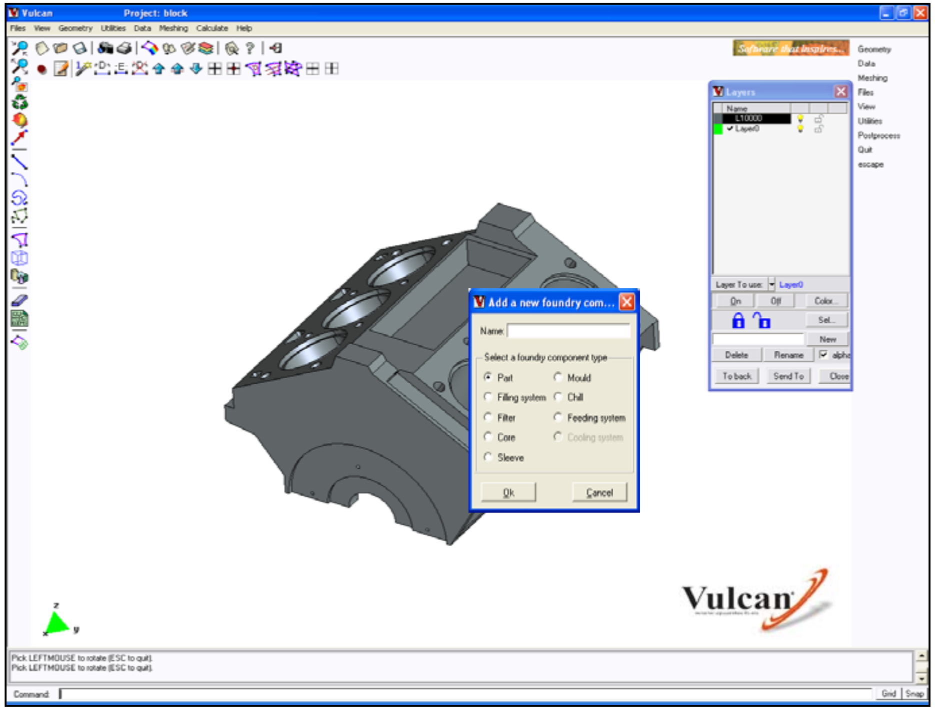
VULCAN User Interface

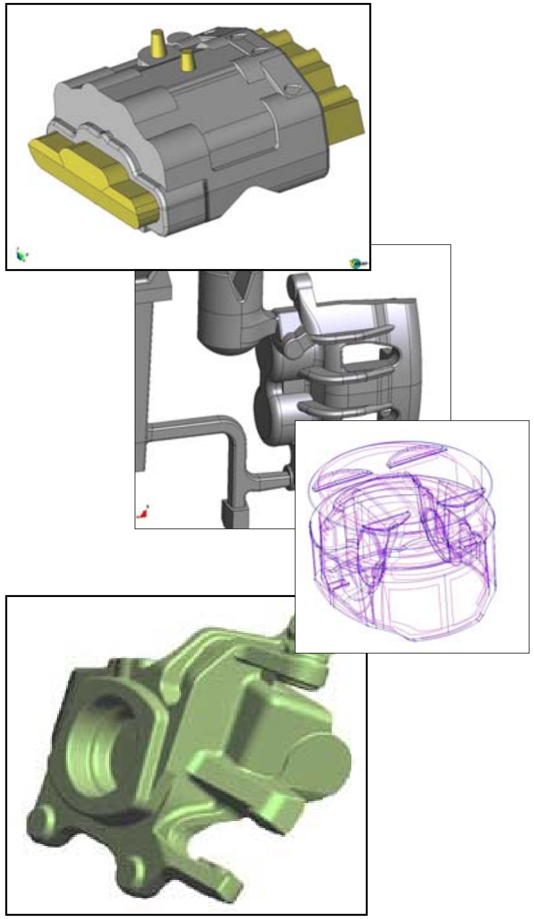
Fully integrated software environment
User-friendly and fully menu-driven

- **Pre-processing: model set-up**
  - **CAD data import**
  - **Repairing CAD data tools**
  - **Meshing**
  - **Comprehensive material data-base**
- **Multi-physics solvers: FE based**
  - **Flow solver coupled with thermal analysis and free-surface identification**
  - **Coupled thermo-mechanical solver including phase-change module**
  - **Stress module for the load analysis after manufacturing process**
- **Post-processing: result analysis and reporting**
  - **Contour-fill, contour-lines, graphs, vectors display, etc.**
  - **Sectioning and cutting planes**
  - **User-defined macros**
  - **Snap-shot, photos, animations and video-clip integrated tools**

VULCAN User Interface

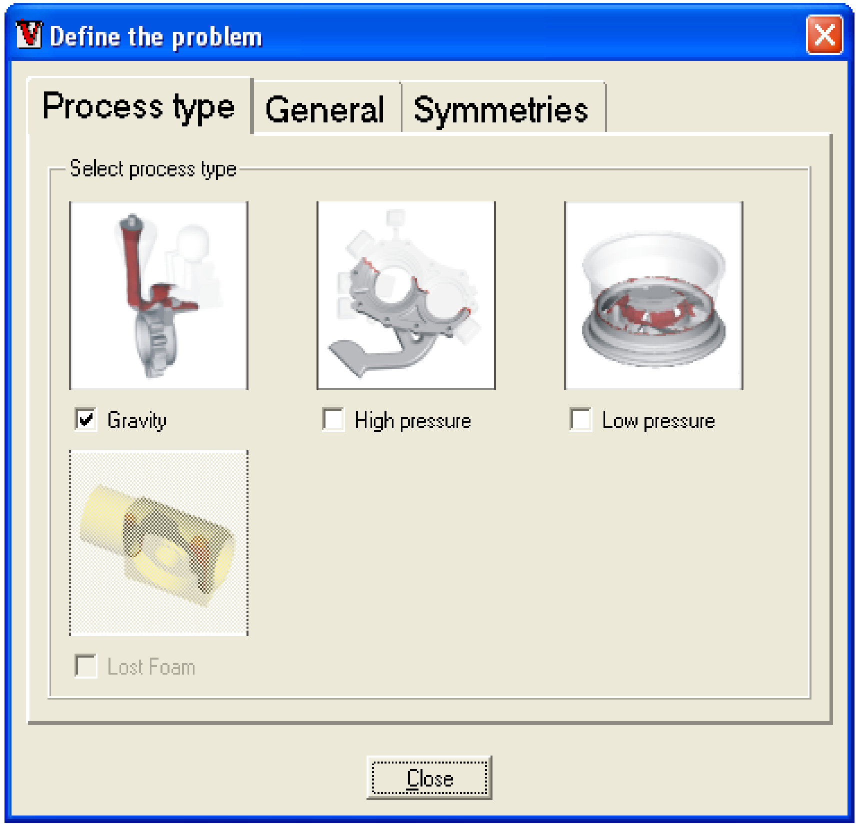
- **User-friendly and fully menu-driven**





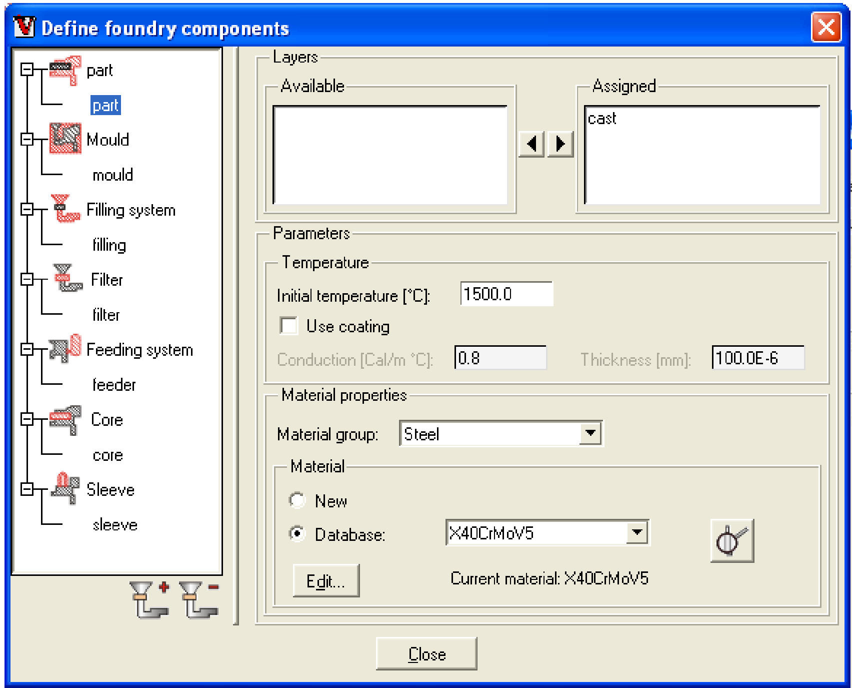
VULCAN User Interface

- New generation, fully integrated software environment
- Step-by-step menu-driven process definition
- Default setting of most analysis parameters
- Fully automatic boundary conditioning and constraining
- On-line tutorials and help
- Customizable software interface

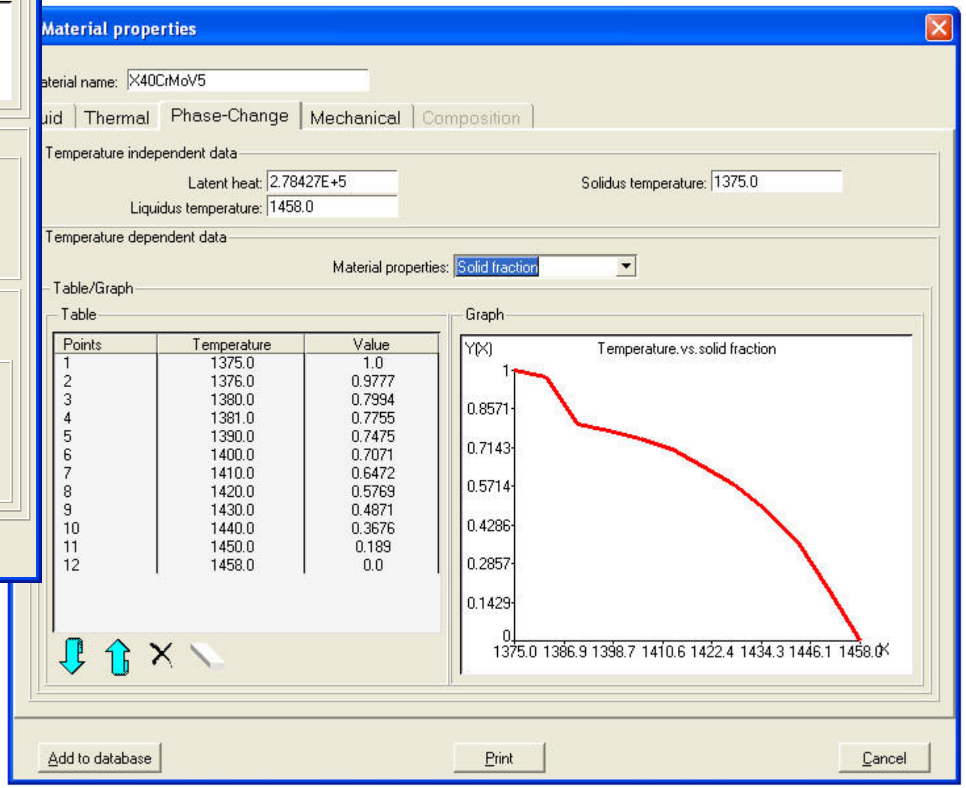


VULCAN User Interface

- **Definition of foundry component**



- **Material data-base**



Conclusions

- Mixed u/p formulation has been introduced to deal with incompressibility behaviour typical of the liquid phase and purely deviatoric plastic deformations
- Continuum transition from liquid-like to solid-like behaviour is achieved introducing a thermal j2-viscoplastic model that reduces to a purely viscous model when material is in liquid-like phase.
- Enthalpy formulation is used to solve the balance of energy equation including phase change
- Ill-conditioning induced by mechanical contact formulation has been smoothed introducing a block-iterative algorithm.
- Optimization toll based on genetic algorithms is available to enhance the numerical solution by an inverse analysis technique.
- Accurate simulation of casting process is achieved.
  Commercial version of the code is available: http://www.quantech.es