Hydration-based multi-physics modelling of cementitious materials for 3D printing

From simulation to process and mix design optimization

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Context and motivation

- **Extrusion-based 3D printing** with cementitious materials is a growing technology allowing for optimal use of material and freedom of form
- However, there is **a lack of simulation tools** able to predict stability during printing as well as durability in the service life
- Cementitious materials **involve coupled mechanisms** which cannot be ignored
- **Detailed simulation** of 3D printing with cement-based materials could **help determine key parameters** within the process or material mix designs

A simulation framework for 3D printing of cement-based materials

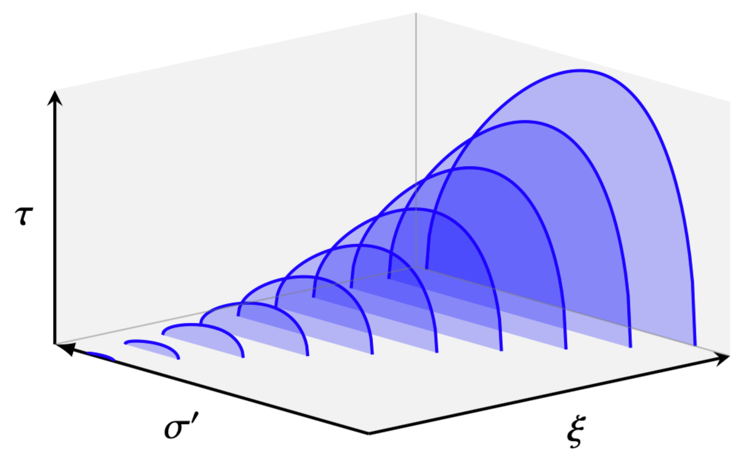
Material Model

Fully coupled thermo-hydro-chemo-mechanics :

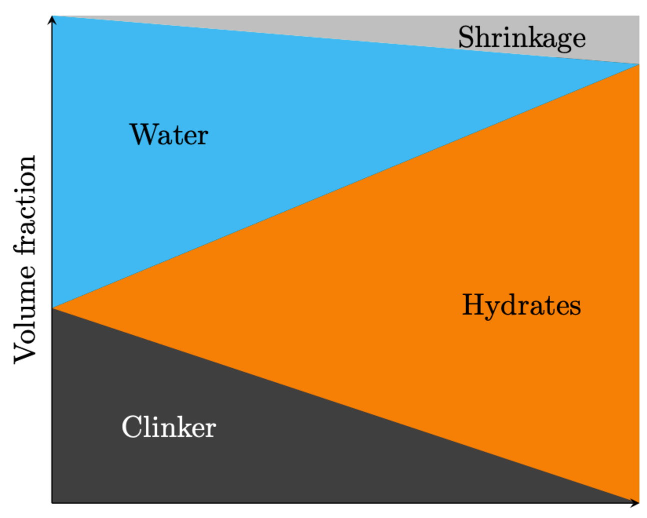
$$(\underline{\sigma}, m_f, S, \mathcal{A}_i) = f\,(\underline{\varepsilon}, p_f, T; \xi_i)$$

Driven by **hydration** reactions ξ_i :

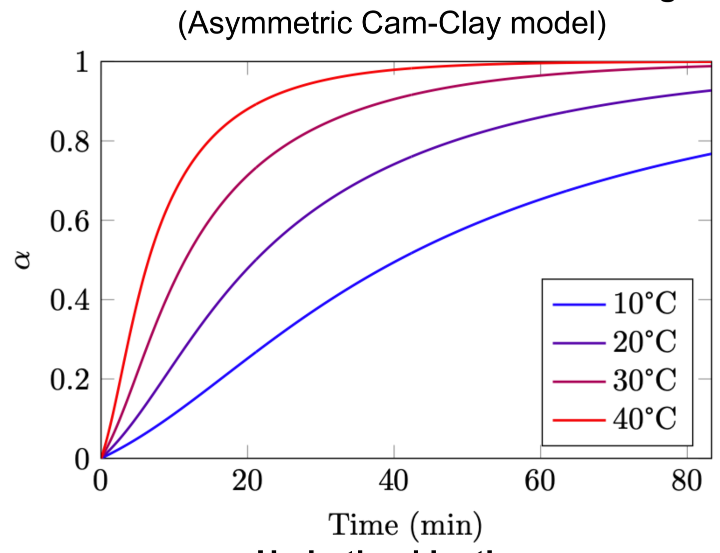
- Hydration-dependent **poroelasticity**
- **Evolving pore structure** affecting the retention curve and permeability
- **Unsaturated state** affecting permeability and hydration reaction rates



Yield surface with chemical hardening
(Asymmetric Cam-Clay model)



Water consumption and shrinkage



Hydration kinetics

External actions

Mechanical:

- Vertical pressure at the printer nozzle from mortar flow

Thermal:

- Convective heat flux at mortar/air interfaces

Hydro-thermal:

- Evaporation flux at mortar/air interfaces dependent internal and external temperature, relative humidity and wind speed

3D simulation of a vase during printing

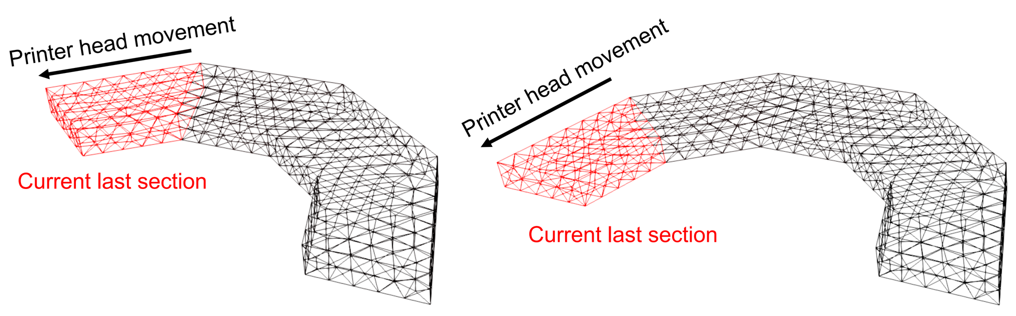
Magnified displacements

Finite element process modelling

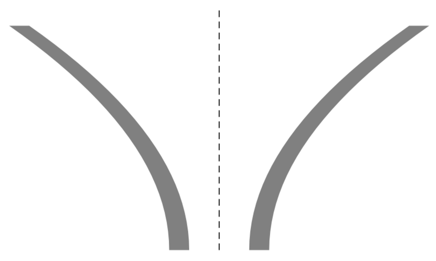
- **Automated reconstruction of mesh** from robot toolpath and lace section
- **Mesh-conforming internal boundaries** for good mesh segmentation at each time step
- Both 3D et 2D axisymmetric methods

Modelling of the printing process through **sequential addition of material**:

- Each time step has a different mesh
- Results of previous time steps are used as initial state for the next



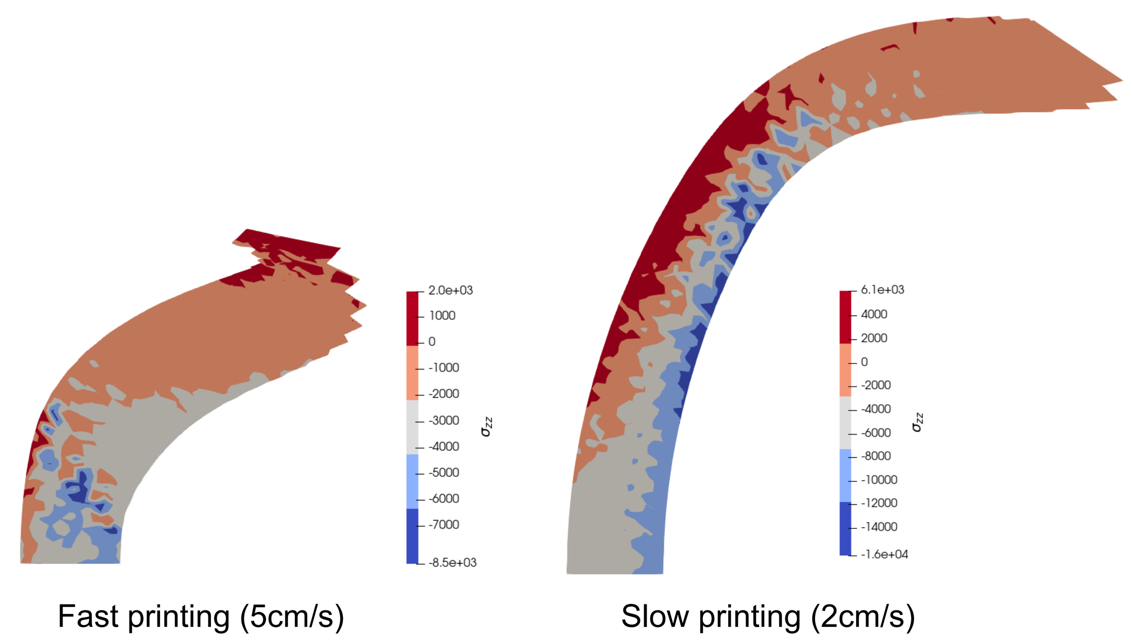
Plastic failure modes – Printing speed dependence



Printed geometry (axisymmetric corolla)

40 Layers height

- **Plastic failure** does not always occur at the bottommost layer
- It is then **hard to use simple analytical tools** to predict plastic collapse of general object, hence the **need for effective simulation** frameworks

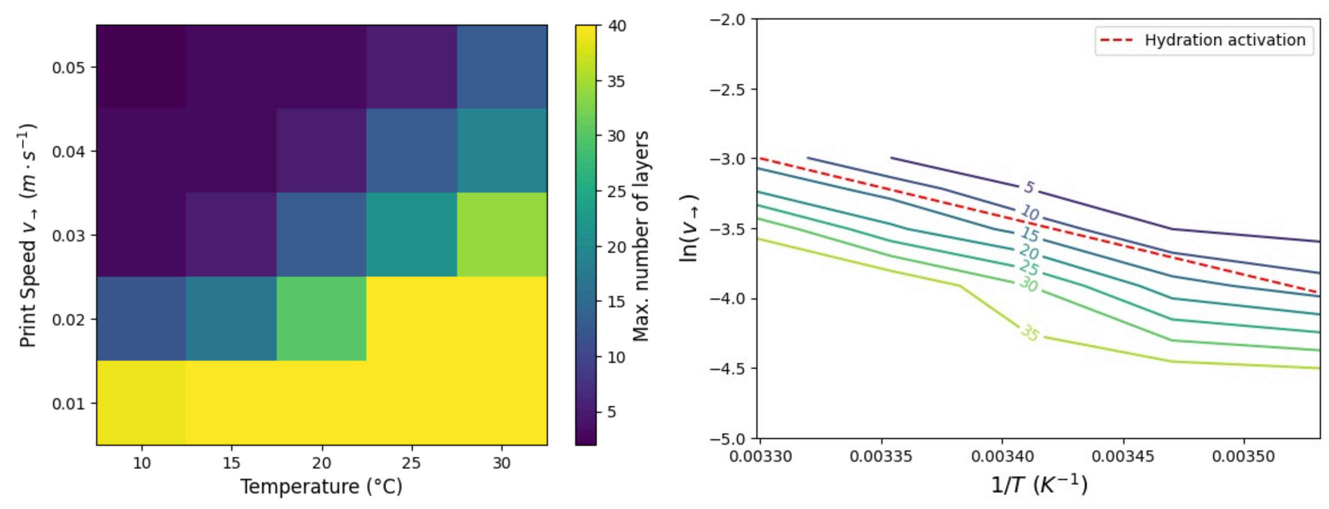


Magnified displacements showing plastic failure mechanisms
(Colour is vertical stress)

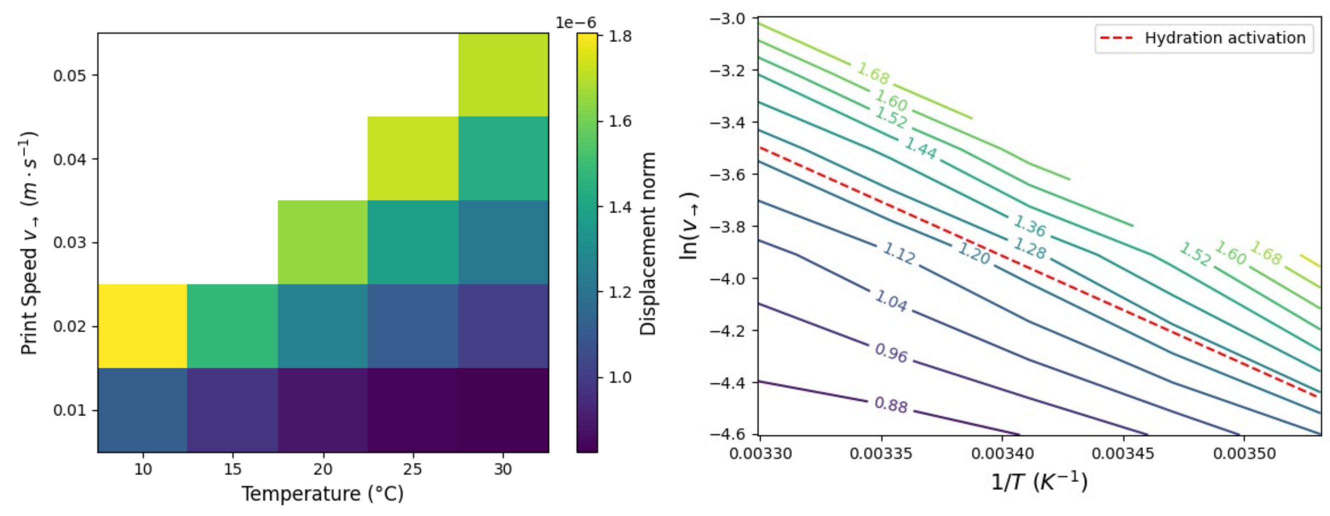
Temperature/print speed effects and trade-off

Printing at different temperatures impacts stability and accuracy of the printing due to modified hydration kinetics:
Can we make up for this impact by adequately modifying the printing speed ?

Decreasing the print speed can allow to retain the maximum number of printable layers at **lower temperatures**, while at higher temperatures one can print faster



The same effect is also true for deformation of the printed object. Modifying the print speed according to the temperature can enable to retain the same level of deformation.



- This effect could be seen as **thermo-activated**:

$$v_\rightarrow(T) \simeq v_\rightarrow(T_0)\exp\left(-\frac{E_A}{R(T-T_0)}\right)$$

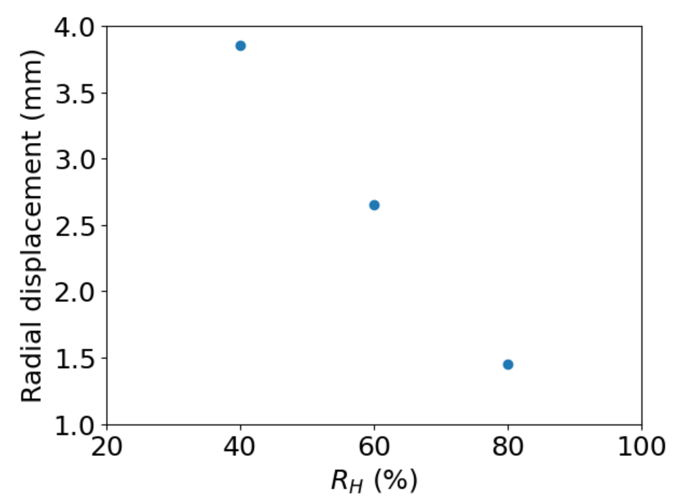
- It has been verified on several geometries that the **activation energy E_A can be taken as that of the hydration reaction** (right-side graphs above) : it **could be used as a rule of thumb for practical applications** such as outdoors printing.

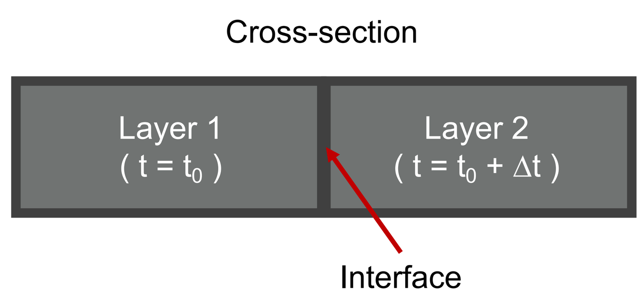
Drying: shrinkage and degraded properties

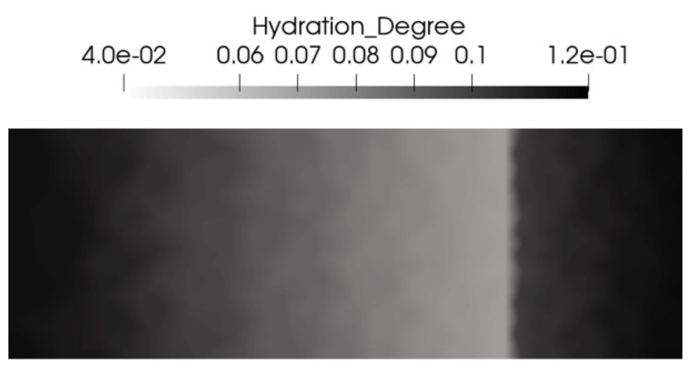
- Water **evaporation flux model** at free surfaces from relative humidity and water vapour saturation pressure taking temperature into account:

$$\phi_{evap} \propto \left(p_{sat}(T_{mat})R_{h,mat} - p_{sat}(T_{ext})R_{h,ext}\right)\cdot f(v_{wind})$$

- R_H **impacts geometric defects** of printed structures (see right, cylinder of radius 15 cm after 15 hours at different R_H)
- Evaporation at the surface can cause **durability problems**:
  - **Degradation of mechanical properties** near the surface (different from bulk material)
  - **Gradient of properties at the layer interface** for long interlayer times (see below)







Layer Interface

Conclusions and perspectives

- Showcased is a **new framework for concrete 3D printing simulation** based on a coupled **multiphysics material model** along with a **finite element** tool handling **sequential deposition of the material** as well as external actions during printing
- This framework allows the investigation of **several interesting mechanisms** which are worth exploring further, such as the **effect of room temperature** on printing conditions or influence of **relative humidity** on early shrinkage of print pieces
- **Experimental comparison** with imaging methods on live printings could allow for a validation of the framework along with a fine-tuning of certain model parameters

References

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