Development of an open-source-based framework for multiphysical crystal growth simulations

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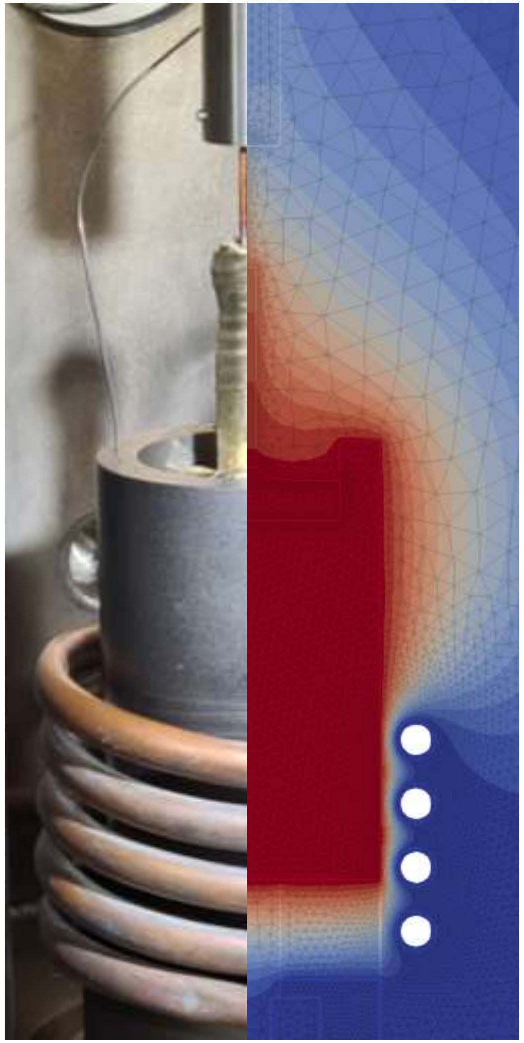
Content



Motivation

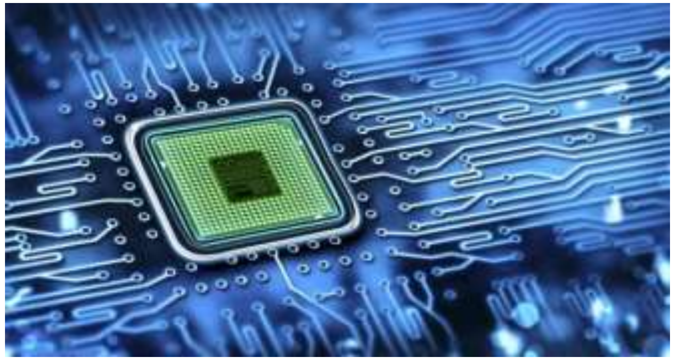
Simulation concept

Transient heat transfer simulation

Possible integration of FEniCS

Conclusion

Motivation – Silicon production



http://www.knoda.org/back-history-discovery-very-first-silicon-chip-digital-computers/

https://cen.acs.org/energy/solar-power/Supercharging-silicon-solar-cell/97/web/2019/07

Computer technology, solar energy

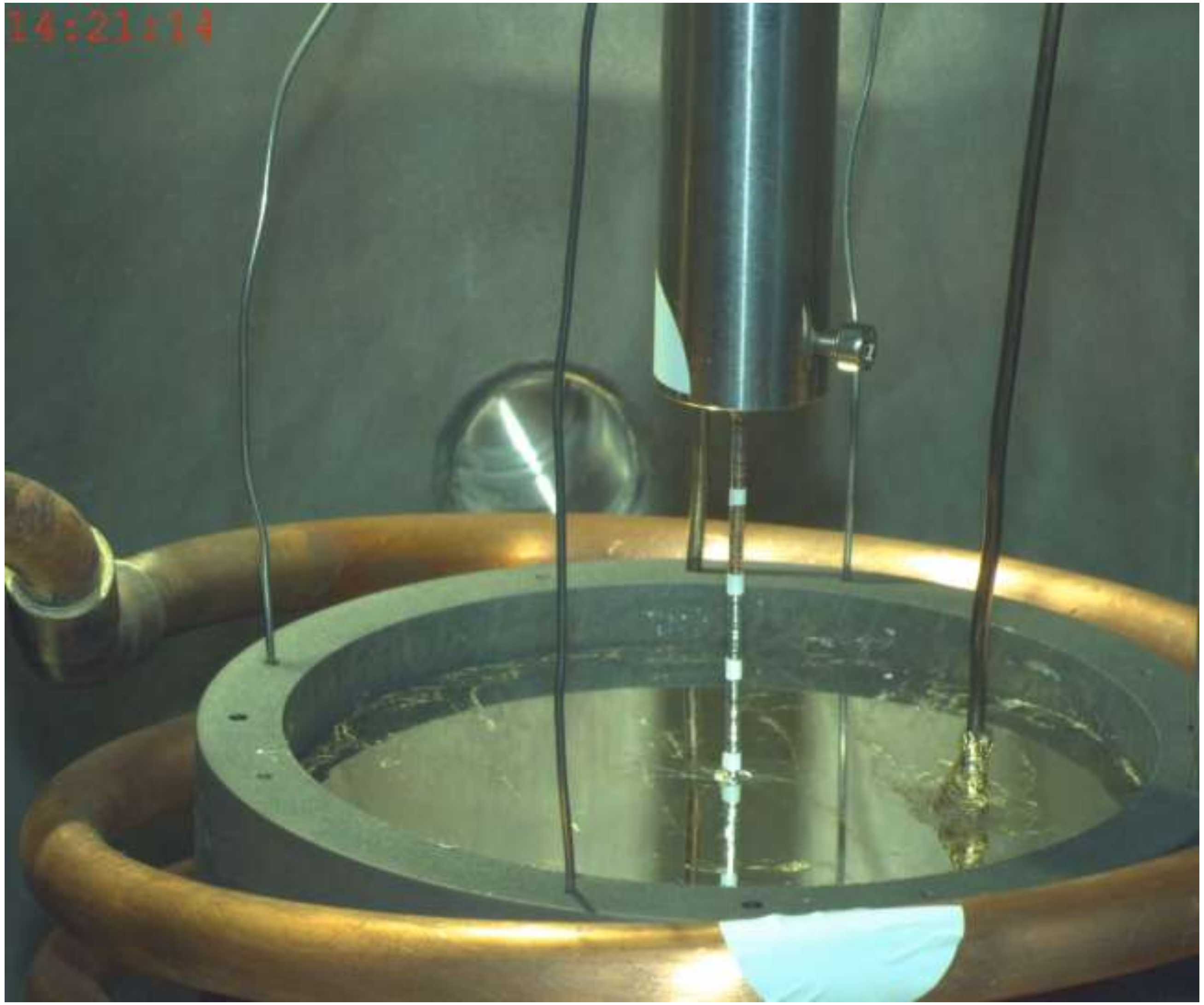
https://www.sciencedirect.com/topics /chemistry/czochralski-process

Silicon single crystal

https://www.pvatepla-cgs.com/anlagen/czochralski/

Czochralski growth furnace

Motivation



Model experiments

Simplified geometry and material

Materials

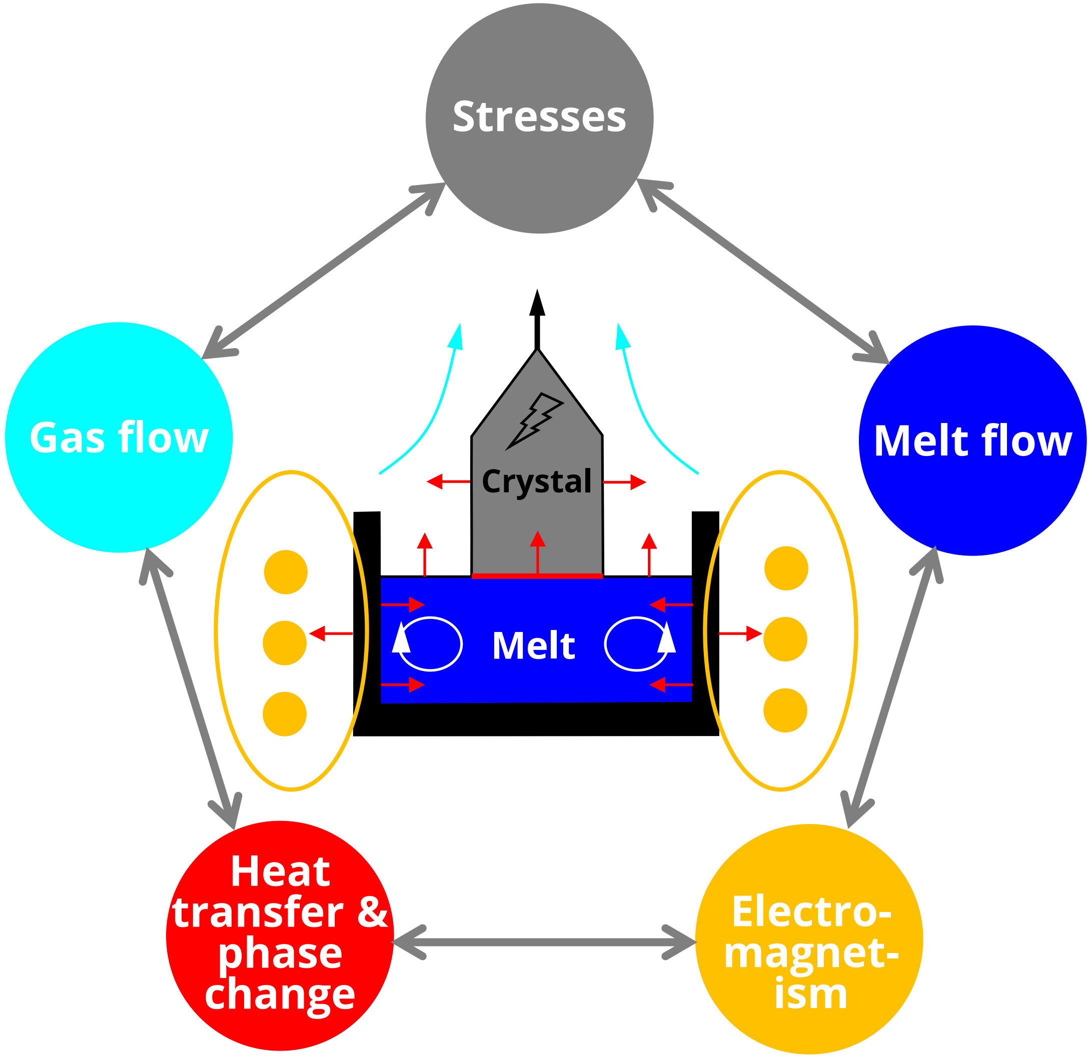
- Tin, $T_{melt} = 232°C$
- Bismuth, NaNO3, …

Conditions

- Air atmosphere
- Vacuum

Measurements

- Temperatures
  - Thermocouples, Pt100
  - IR Camera
  - Pyrometer
- Electromagnetism
  - Heating power
  - Magnetic field
- Flows, thermal stresses



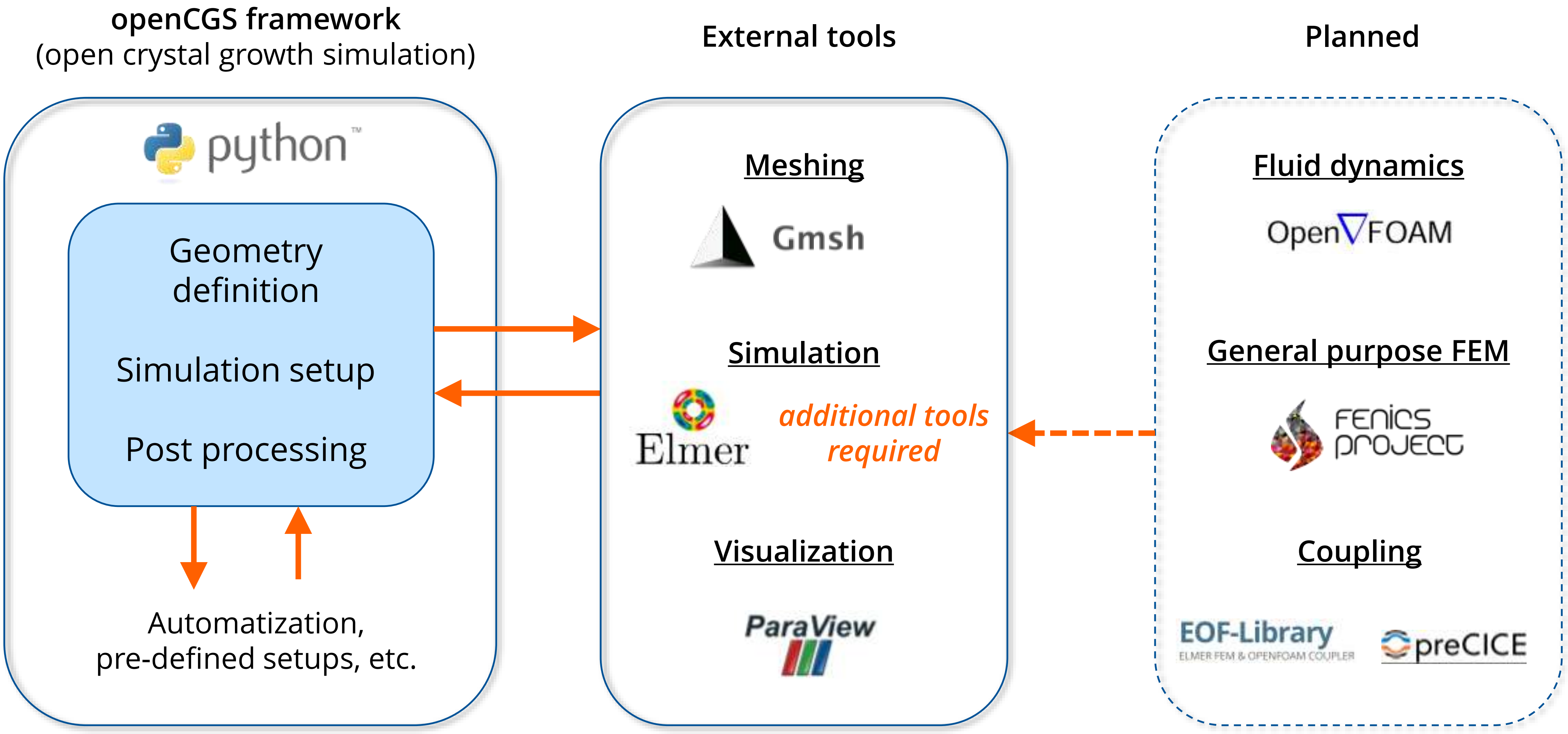
Numerical challenges

- Complex coupled physics
- Moving geometries
- Different timescales
- …

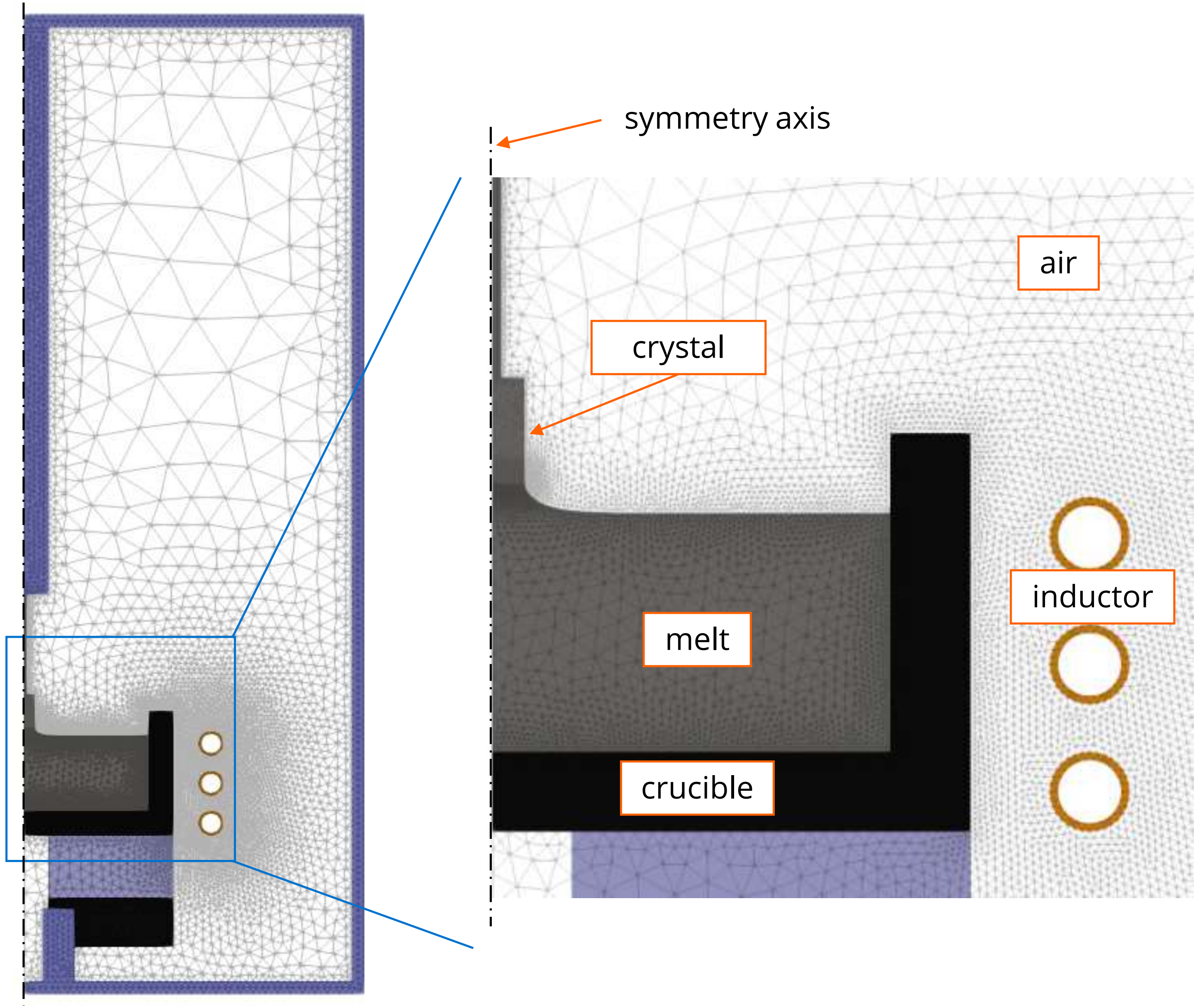
Goals in NEMOCRYS Project

- Validation: Using model experiments
- Open source implementation

Simulation concept



Transient simulation – setup



2D axisymmetric with Elmer

Induction heating (harmonic)

$$\nabla \times \left(\frac{1}{\mu}\nabla \times A_\varphi \boldsymbol{e}_\varphi\right) + i\omega\sigma A_\varphi \boldsymbol{e}_\varphi = j_\varphi$$

Heat transfer

$$\rho c_p \left(\frac{\partial T}{\partial t} + (\boldsymbol{u}\cdot\nabla)T\right) - \nabla\cdot(\lambda\nabla T) = \rho h$$

Phase change (steady-state approximation)

$$q = L\,\rho\,\boldsymbol{v}\cdot\boldsymbol{n}\,,\quad s_y = (y_{j,1} - y_i) + (x_i - x_{j,1})\frac{y_{j,2}-y_{i,1}}{x_{j,2}-x_{j,1}}$$

Radiation (at solid/air boundaries)

$$-\lambda_k \frac{\partial T_k}{\partial \boldsymbol{n}_k} = \sigma_\varepsilon \varepsilon_k \left(T_k^4 - \frac{1}{A_k\varepsilon_k}\sum_{i=1}^{N} G_{ik}\varepsilon_i T_i^4 A_i\right)$$

P. Råback et al.: Elmer Models Manual, CSC – IT Center for Science, 10.11.2020. https://www.nic.funet.fi/pub/sci/physics/elmer/doc/

Transient simulation – procedure

Procedure using Elmer / Gmsh

Steady state simulation

↓ T ↓

Mesh generation (with new L)

↓

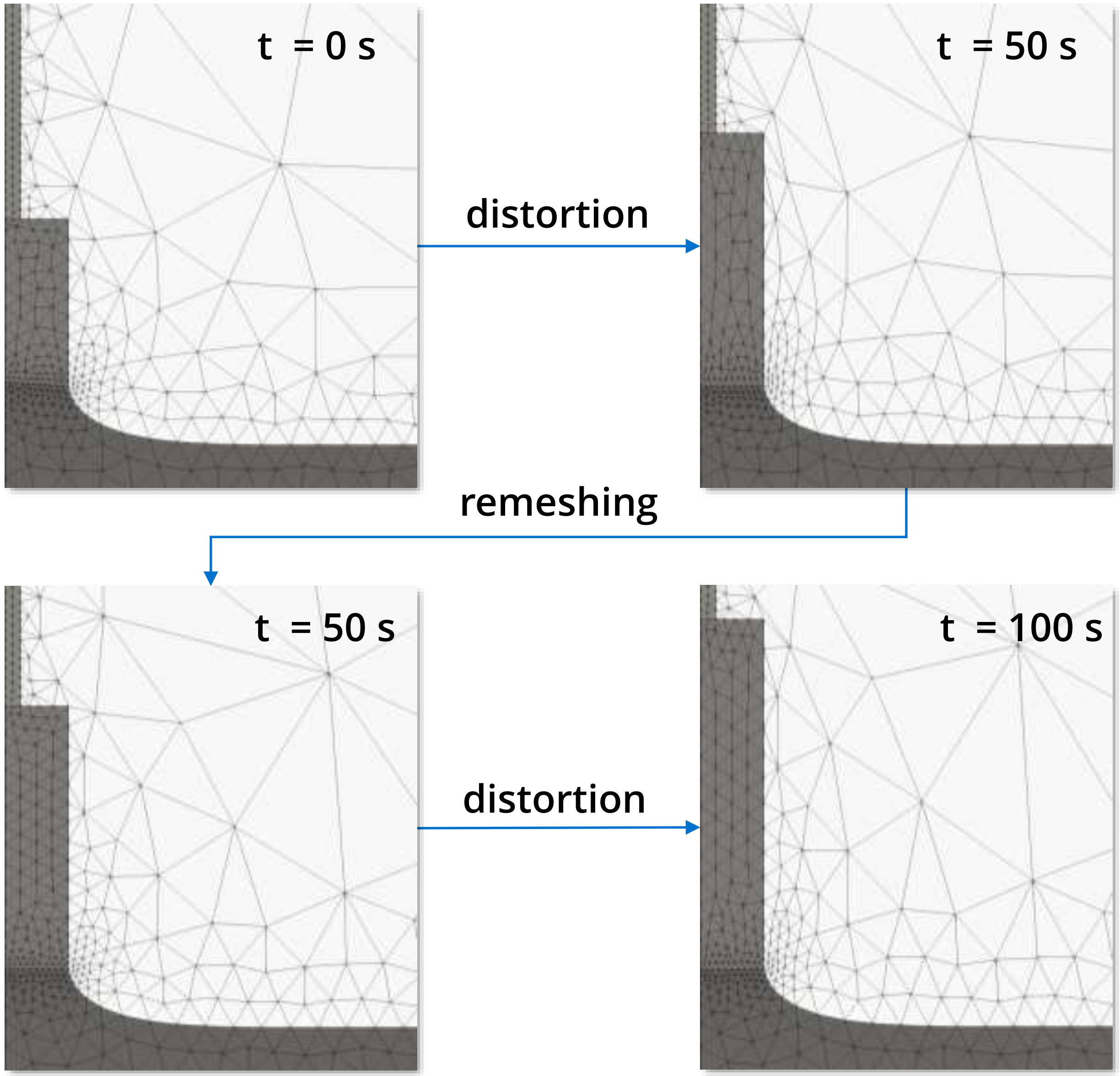
Mesh to mesh interpolation in Elmer

↓

Transient simulation
with mesh distortion

if $l_{crstal} < l_{max}$ (back to mesh generation) | L, T | *else* ↓

Combination of sub-simulations to
one final result in Python



Transient simulation – implementation

Mesh update loop in openCGS
(simplified)

```
sim = SteadyStateSim(geometry,
                     simulation_setup,
                     start_length)
sim.execute()

while start_length < max_length:
    sim = TransientSim(geometry,
                       simulation_setup,
                       start_length,
                       length_increment,
                       sim)
    sim.execute()
    start_length += length_increment
```

User input: Two functions
(simplified)

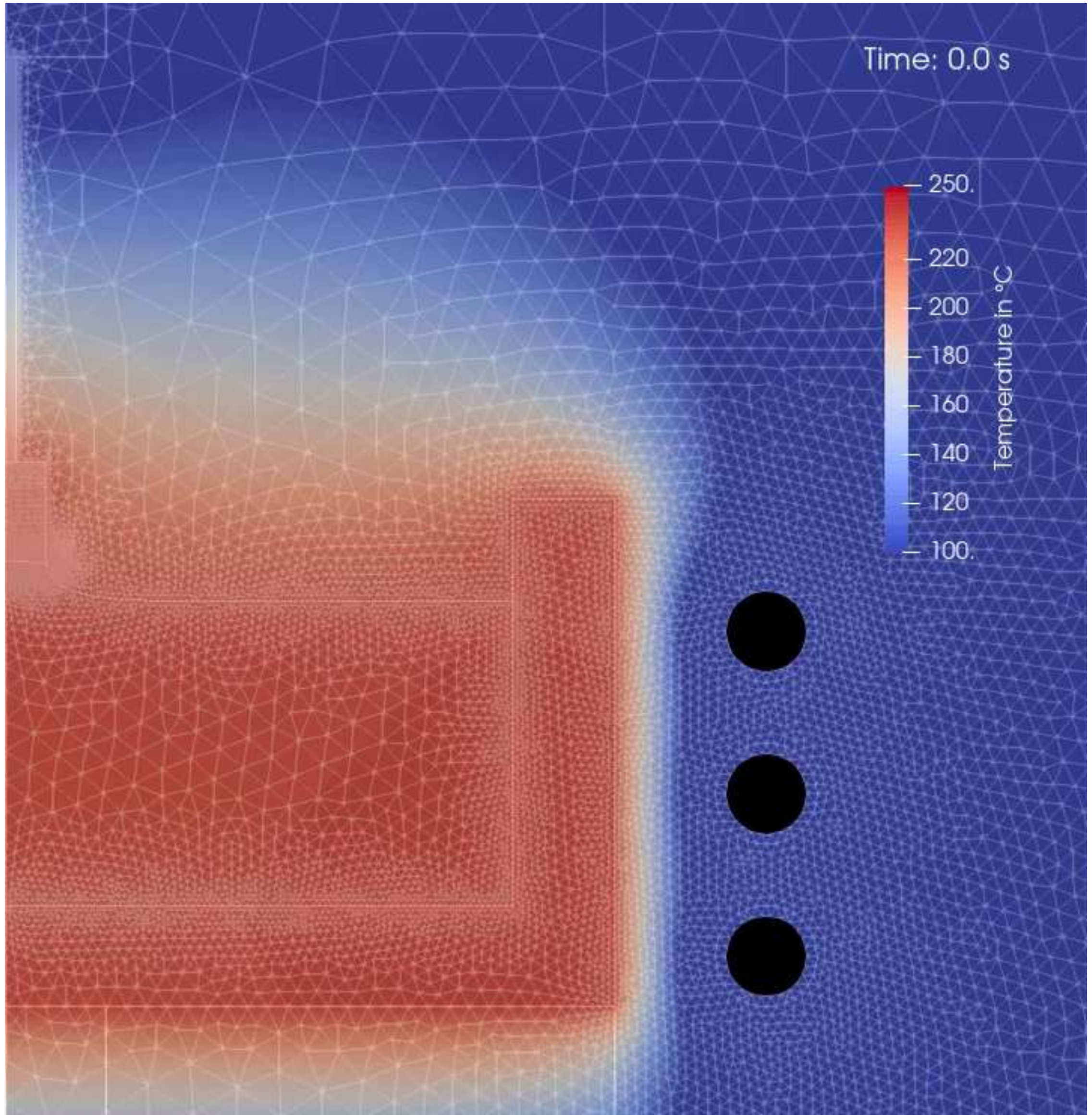
```
from opencgs import geo, setup


def geometry(crystal_length):
    geo.crystal(crystal_length, ...)
    geo.crucible(...)
    geo.melt(...)

    ...  # boundaries, mesh sizes


def simulation_setup(...):
     setup.add_crystal(...)
    ...  # bodies, boundaries
```

Transient simulation – results



Numerical

- Simulation numerically stable
- No visible errors introduced by mesh update

Physical

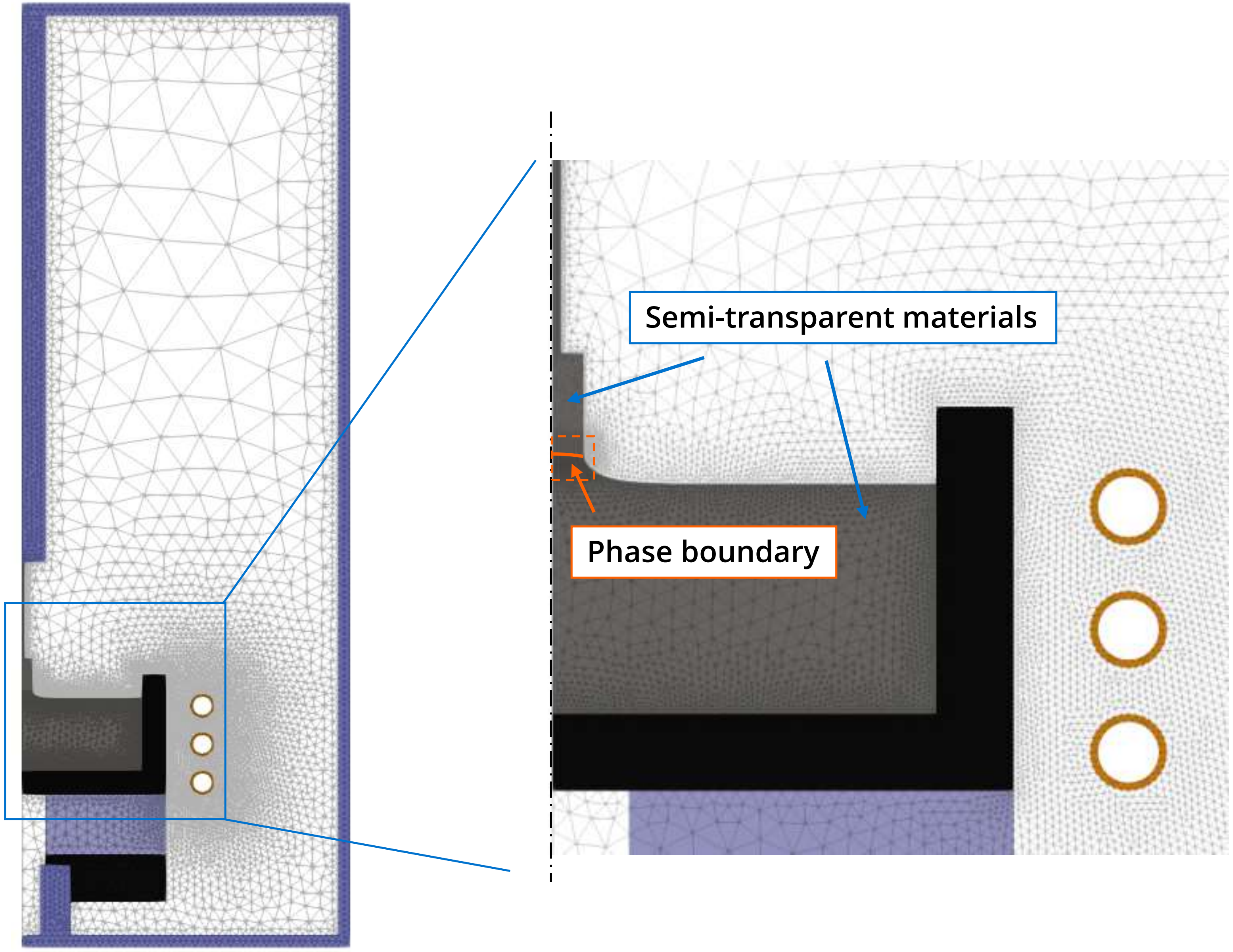
- Increase in temperature with crystal length, corresponds to experiment
- Validation ongoing: Convective cooling of crystal, etc.

Future challenges

- Variable crystal diameters

→ New models required

Possible integration of FEniCS



Need for advanced models

- Phase boundary modeling
  - Growth in axial and radial direction
  - Interaction with process control
- Semi-transparent materials
  - Internal radiation
  - Internal absorption

Possible implementations

- Coupling to Elmer (preCICE)
- Complete solver in FEniCS – radiation model required!

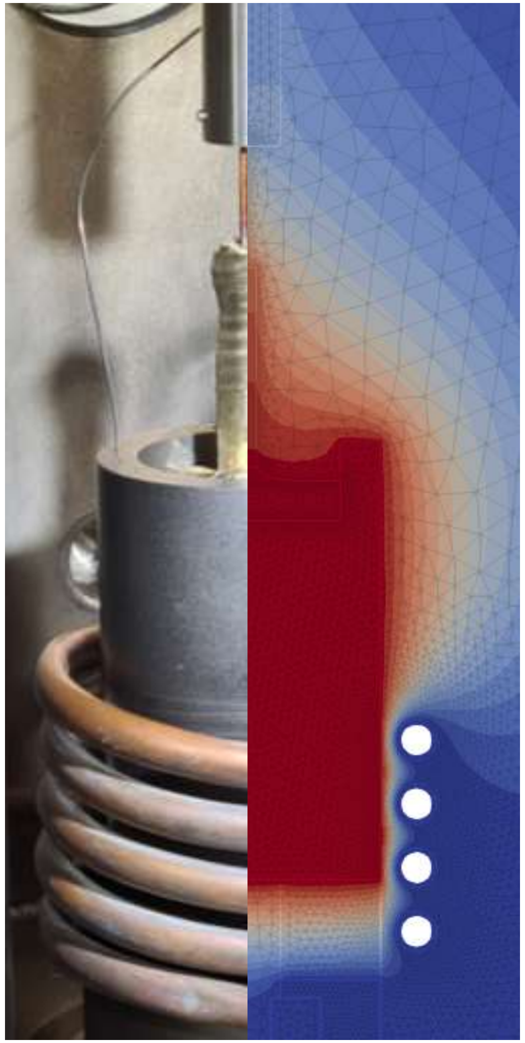
Conclusion

Transient thermal CZ growth simulation implemented

- Python-based framework using Elmer and Gmsh
- Limited to constant crystal diameters

Possible integration of FEniCS

- Coupling to Elmer using preCICE: Under development
- Complete solver in FEniCS: Radiation model required



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