Czochralski Growth of Ge Computed by Using the Finite Element Tool Elmer

Wolfram Miller

Leibniz Institute for Crystal Growth Berlin

Member of Leibniz Association

Outline

- Some introduction:

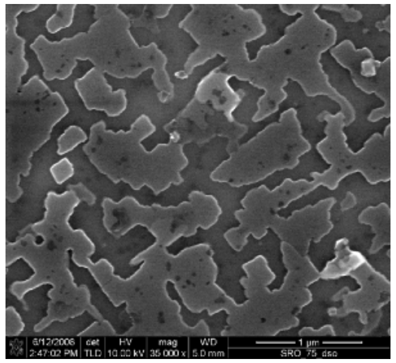
  From Sand (of the desert) towards quantum dots

  Crystal Growth
- Motivation: Ge crystals for detectors
- Experiment & Simulations setup
- Solving strategy
- Elmer
- Results & Discussion
- Conclusions

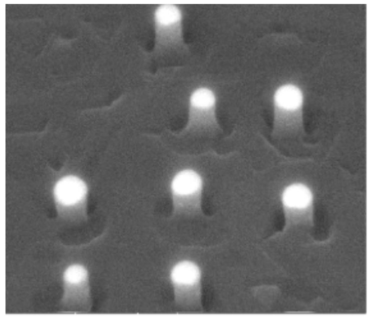
Crystal Growth IKZ

- Bulk crystal growth
  substrates
  bulk for optics (laser, lenses ...)

- Epitaxial / thin film growth

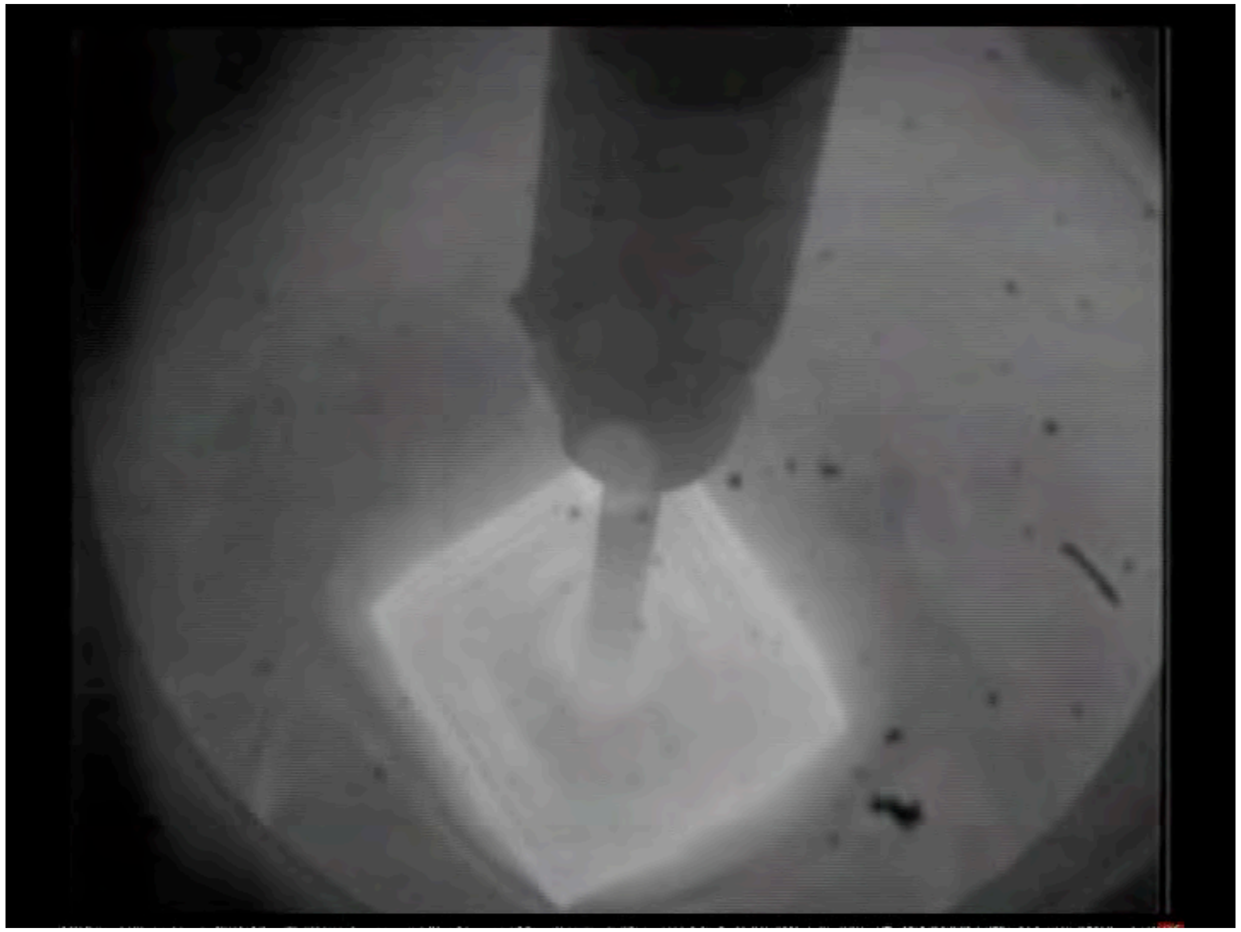


- Growth of nanostructures



Czochralski Growth of Silicon

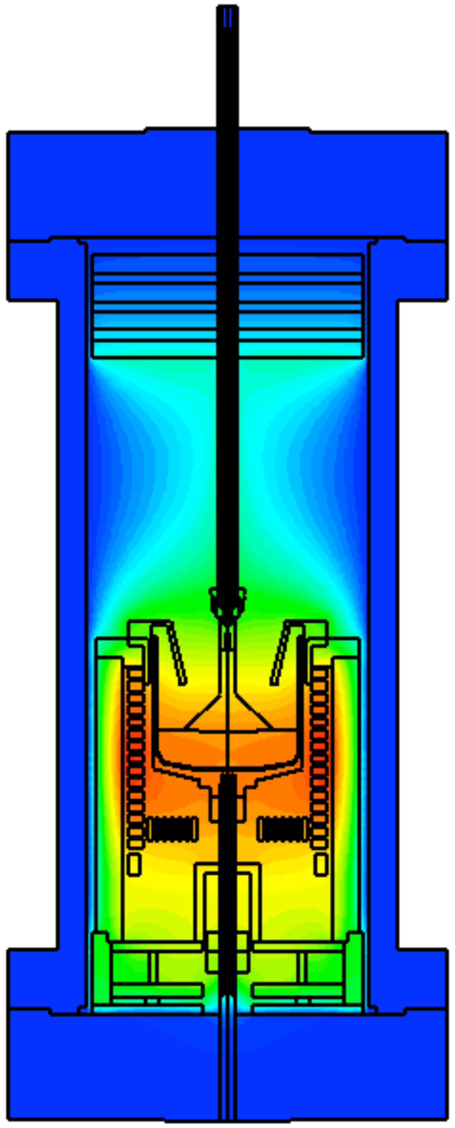
Siltronic AG, Burghausen



Numerical Modelling

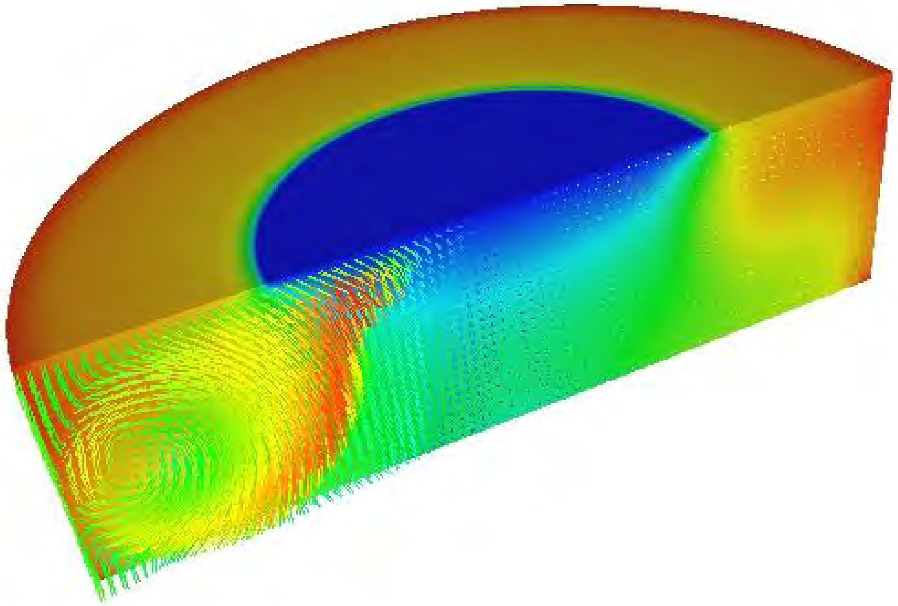
Global 2.5 D

Local 3D



Transfer thermal data

temperature
heat flux



Ge Crystals for Detectors

Projects Gerda & Legend

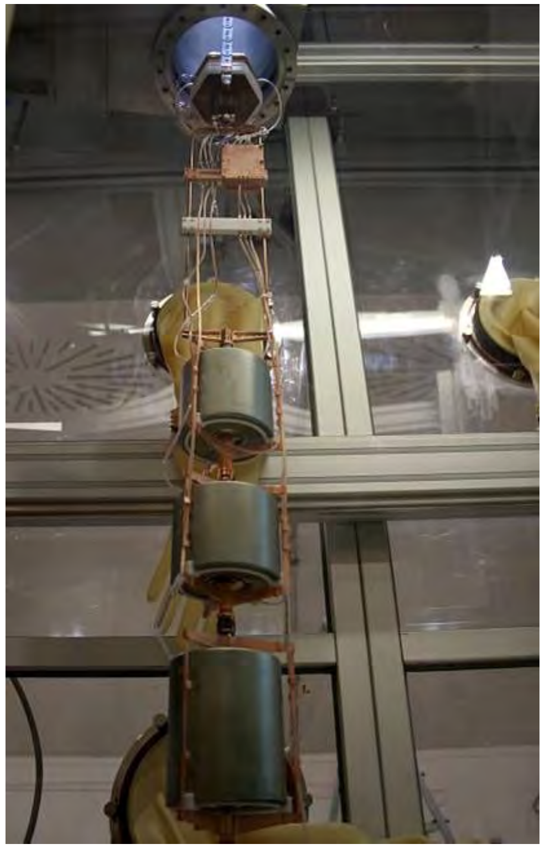
Aim: find neutrinoless beta decay $^{76}Ge \rightarrow {}^{76}Se$

☞ absolute mass of Neutrinos

Experiment at Gran Sasso

30 kg Ge

200 kg scheduled



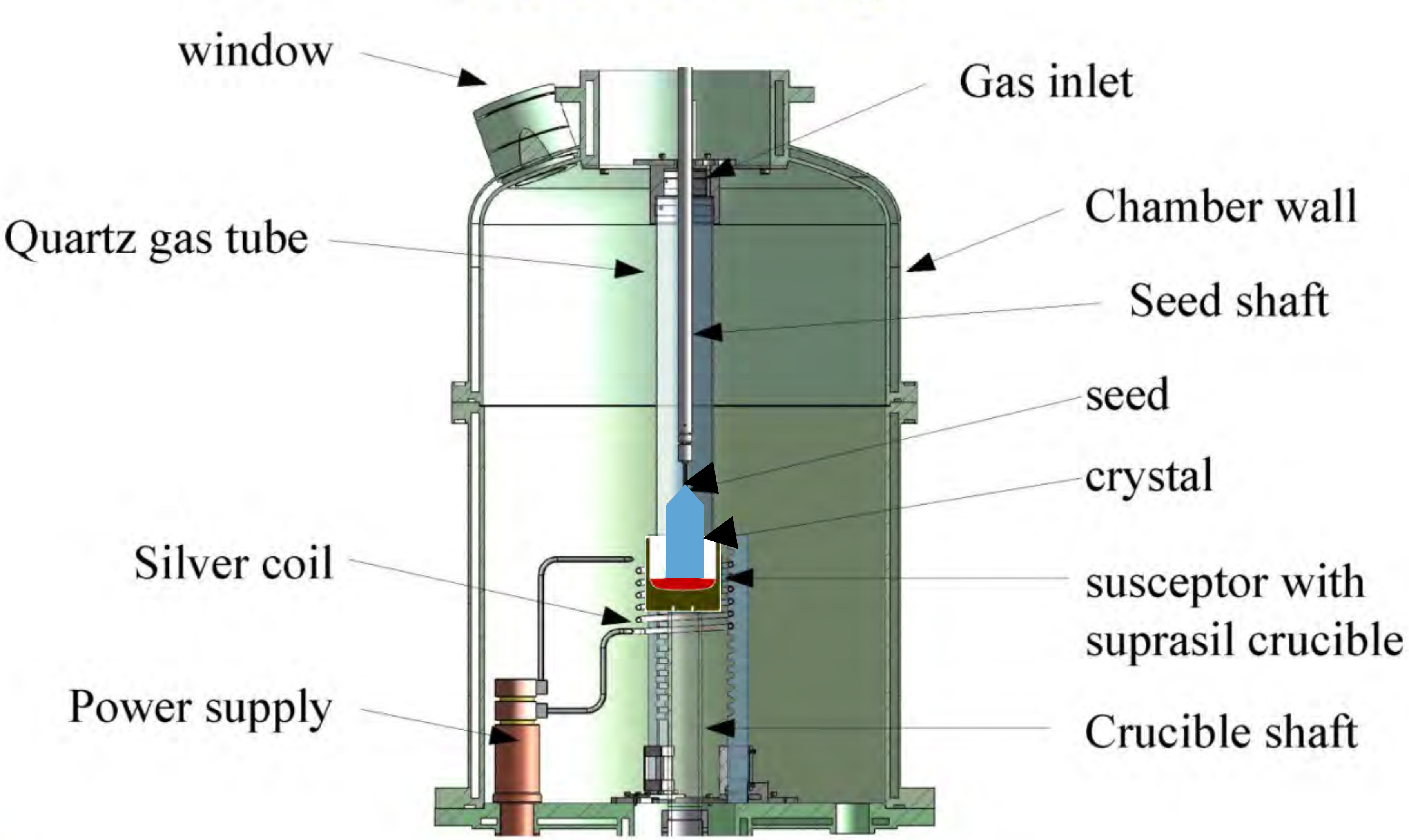
Ge Crystals

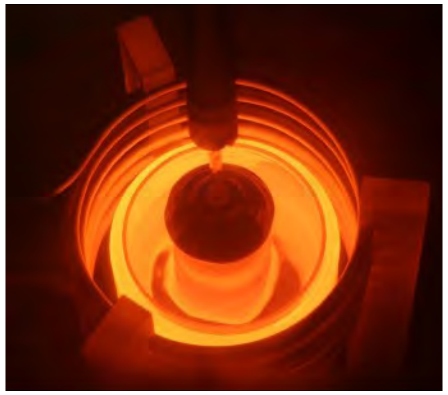
Ge is target and detector

- single crystal
- high resistivity, which means extreme purity
- low density of dislocations (structural defects)

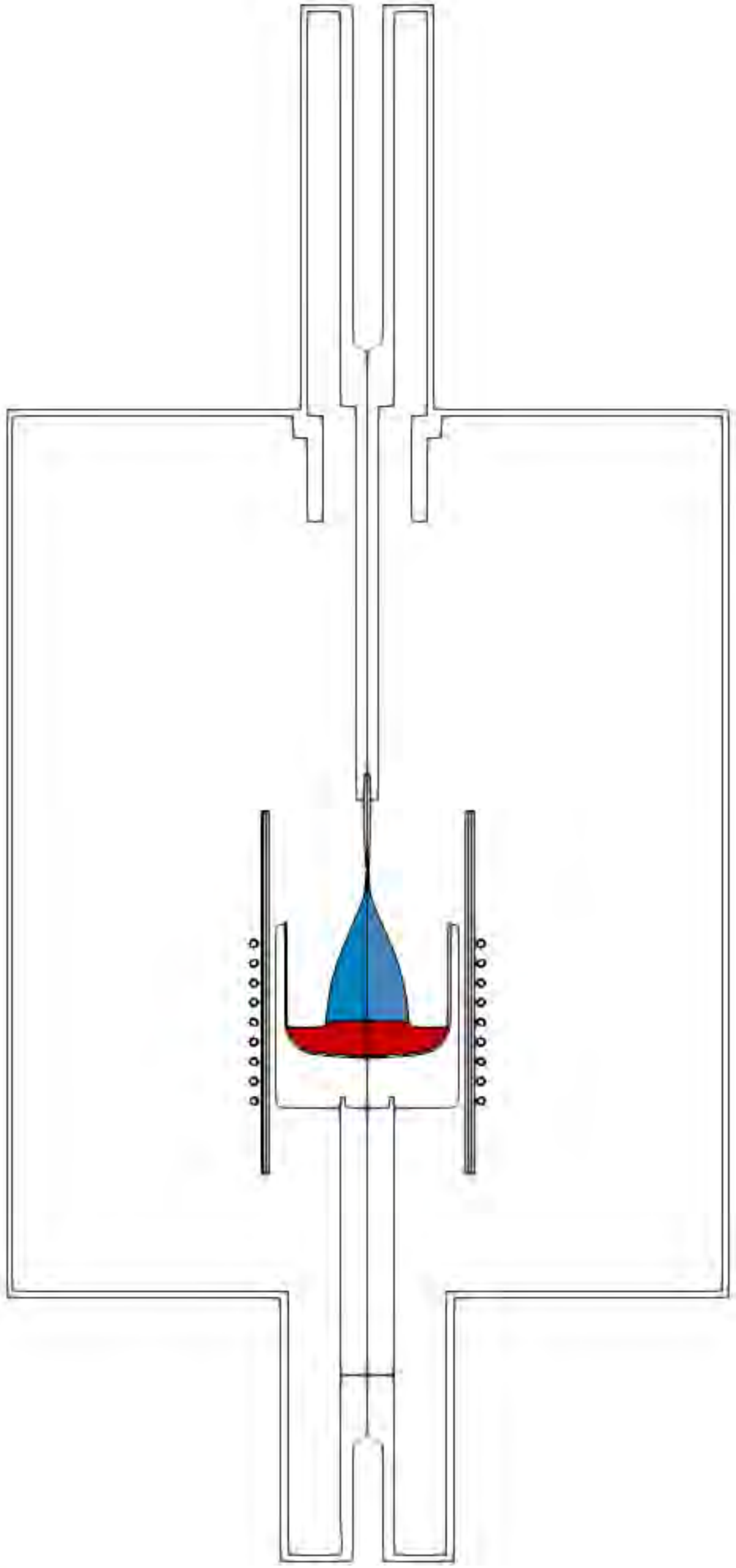
⇨ crystals are grown by Czochralski method with inductive heating

Ge Crystals by Czochralski Growth





Simulation Setup: Physics

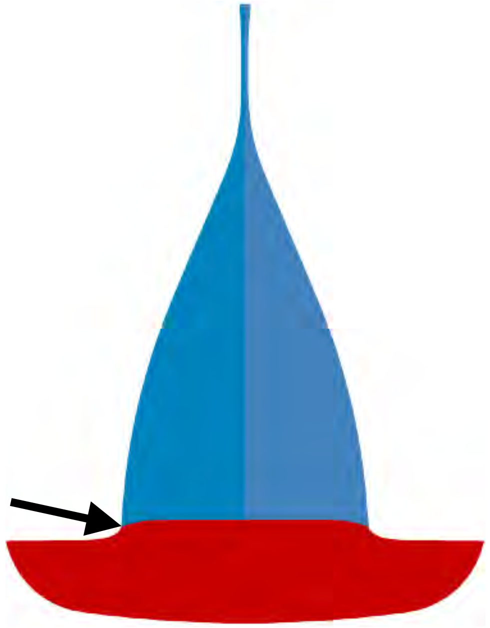


axi-symmetric calculations

- Temperature
  - heat conduction
  - radiation
  - melt convection
  - (gas convection)

  - inductive heating
    control by T_M @ 3PP

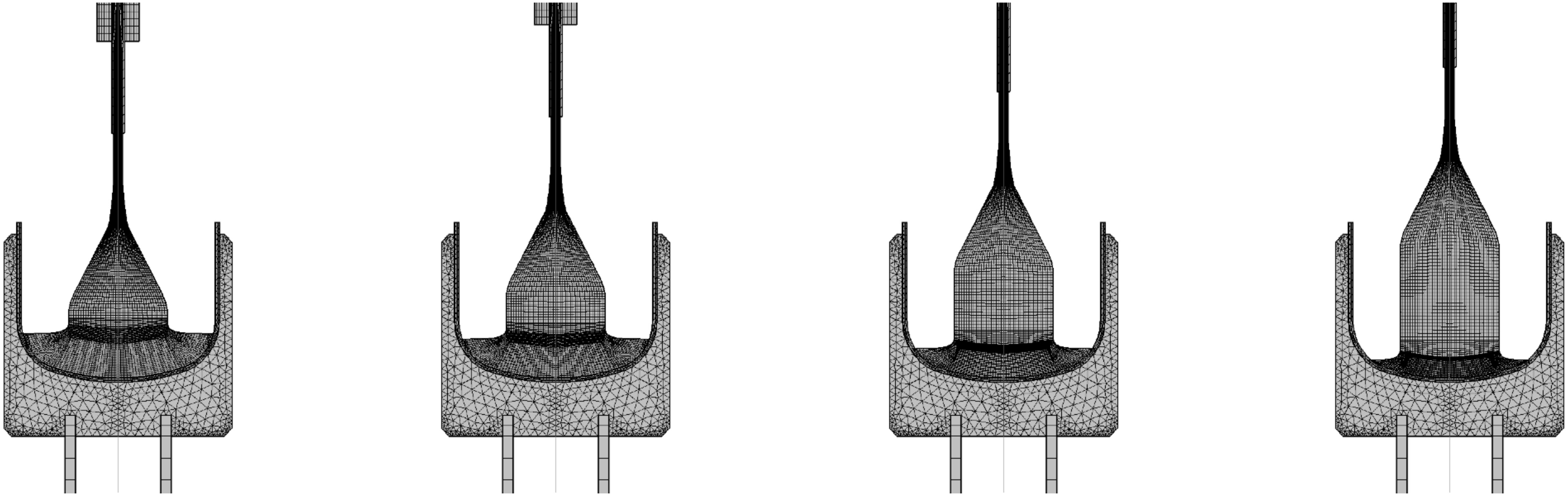
  - solid/melt interface
    - release of latent heat
    - shape



- Stress
  - thermal stress in crystal

Simulation Setup: Process

$v_{pull} = 0.5$ mm/min

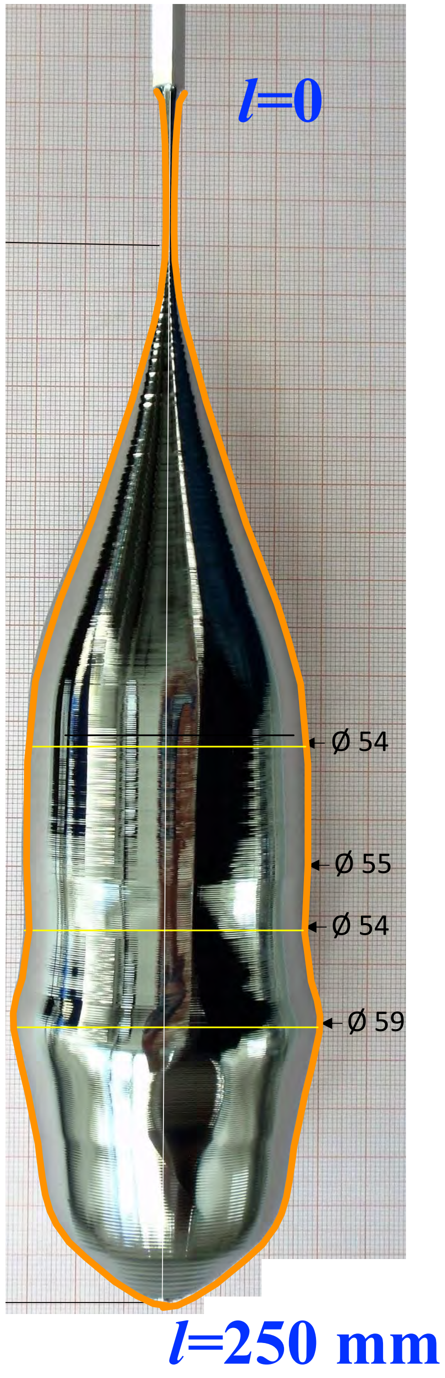


a) Fully transient calculation (with mesh squeezing and elongation)

b) Series of steady-state simulations

Solving Strategy

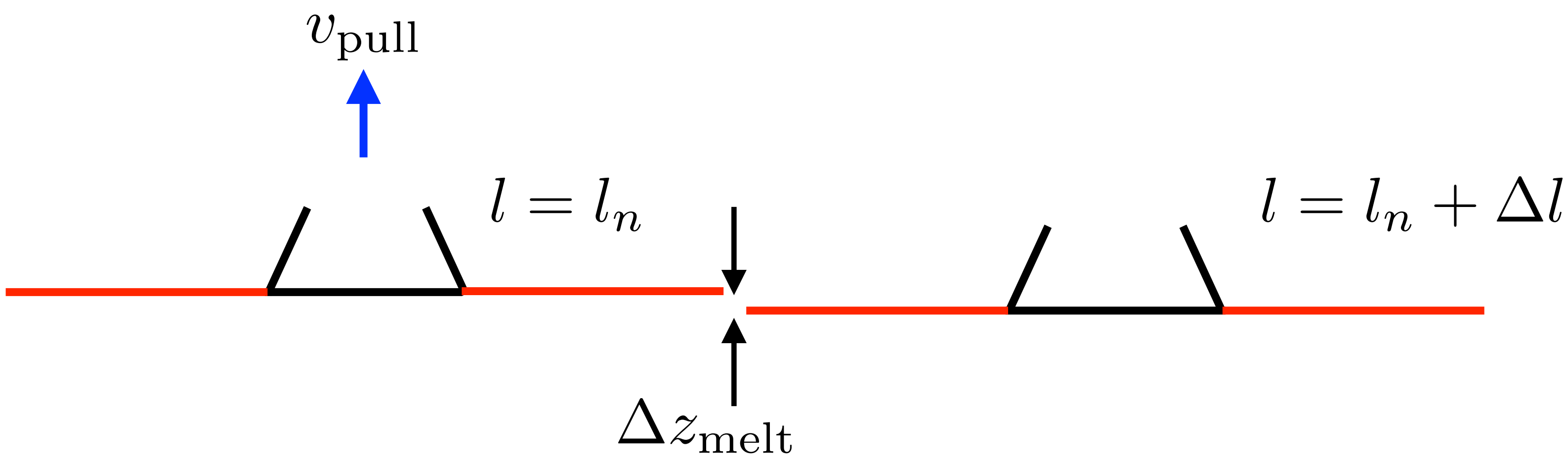
- Crystal Shape given
  a) from experiment
  b) as given input



Solving Strategy

- Perl Script:
  - From $l=0$ in steps of Δl

    ⇨ compute melt height and v_n



$$\Delta l = \Delta z_{\text{melt}} + v_{\text{pull}}\,\Delta t$$

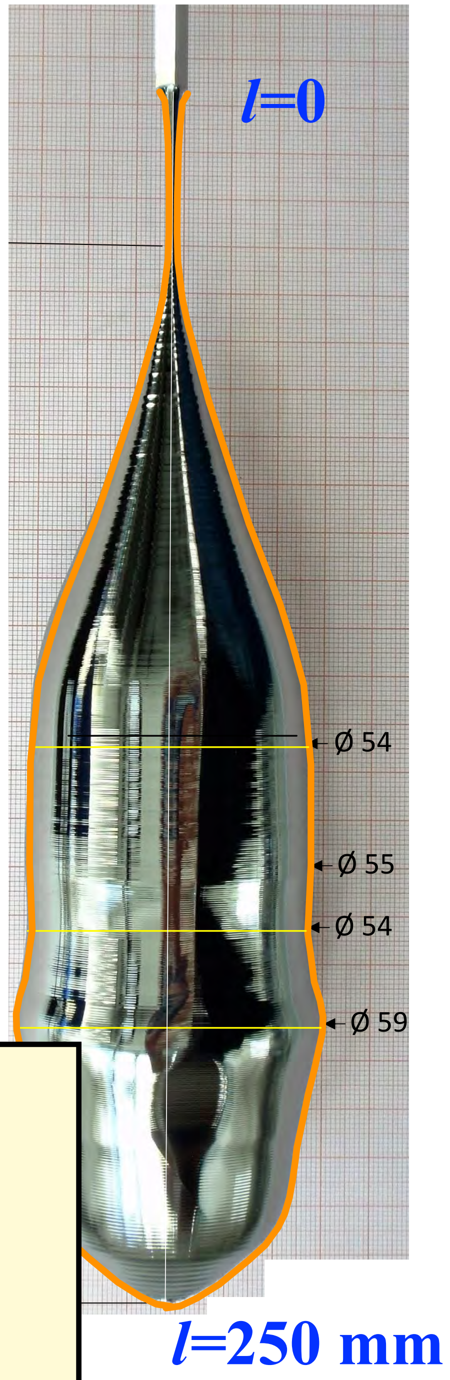
fixed computed fixed

$$v_n = \frac{\Delta l}{\Delta t}$$

heat flux into crystal

$$q = v_n \Delta H$$

latent heat

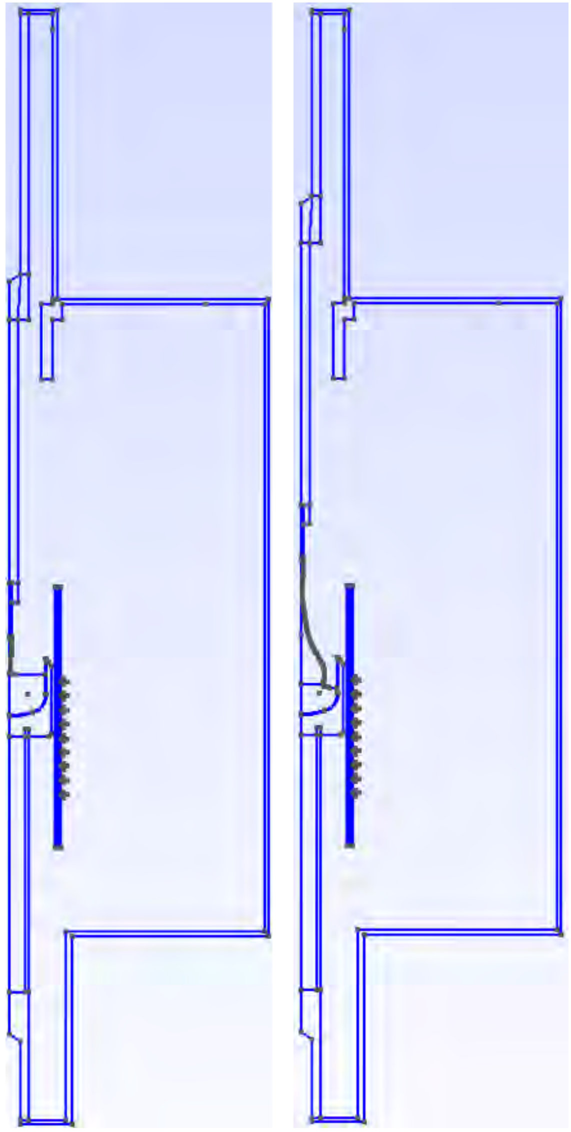


Solving Strategy

- Perl Script:
  - For every Δl n_{step}
    - ⇨ perform a steady-state calculation
      - ✗ geometry (melt, crystal & holder, melt/gas, interface) computed in perl script
      - ✗ mesh by gmsh
      - ✗ computation by Elmer

Solving Strategy

- Perl Script:
  - For every $\Delta t = \Delta l \;\; t_{\text{step}}$
    - ⇨ perform a steady-state calculation
      - ✗ geometry (melt, crystal & holder, melt/gas, interface) computed in perl script
      - ✗ mesh by gmsh (http://gmsh.info/)
      - ✗ computation by Elmer
      - ✗ visualisation by Paraview



Elmer

- FEM multiphysical simulation software
- Developed at CSC, Espoo (Finland) since 1995
- Since 2005 open source
- written in FORTRAN
- Uses MATC for mathematical expressions

https://www.csc.fi/web/elmer

http://www.elmerfem.org/

Elmer

```
!!! melt
Equation 2
  Active Solvers(6) =   1 2 3 9 7 8
End
```

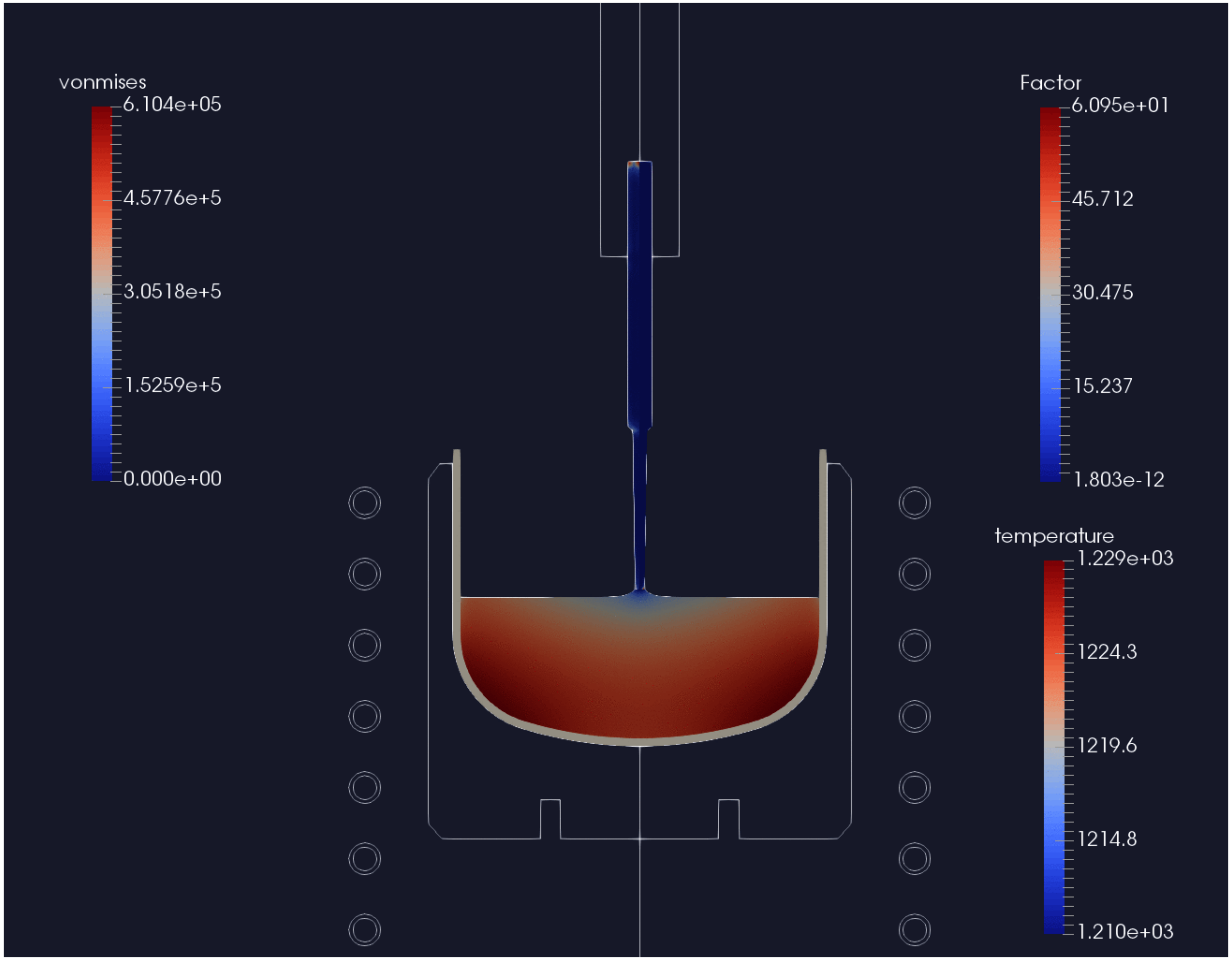
```
Solver 3
 Equation = Heat Equation

 Procedure = "HeatSolve" "HeatSolver"
 Variable = -dofs 1 Temperature

 Temperature Convection Field = Flow Solution Melt [Velocitymelt:3 Pressuremelt:1]

End
```

Result RGZ 39



Melt Convection

Steady state solver

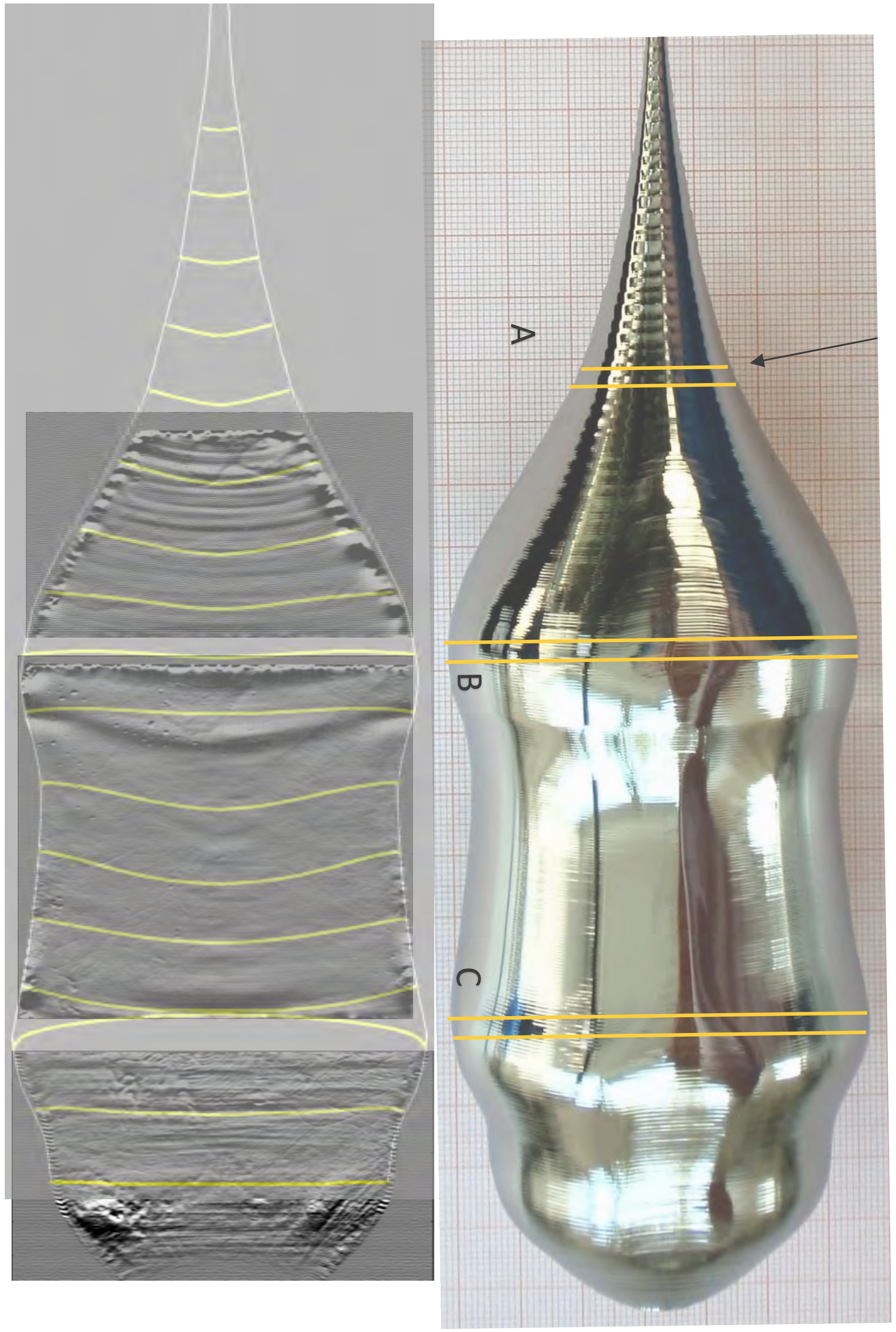
Real viscosity $\mu = 7.44 \times 10^{-4}\ \mathrm{Pa\,s}$

Choosing larger one (finally $\mu = 5 \times 10^{-3}\ \mathrm{Pa\,s}$)

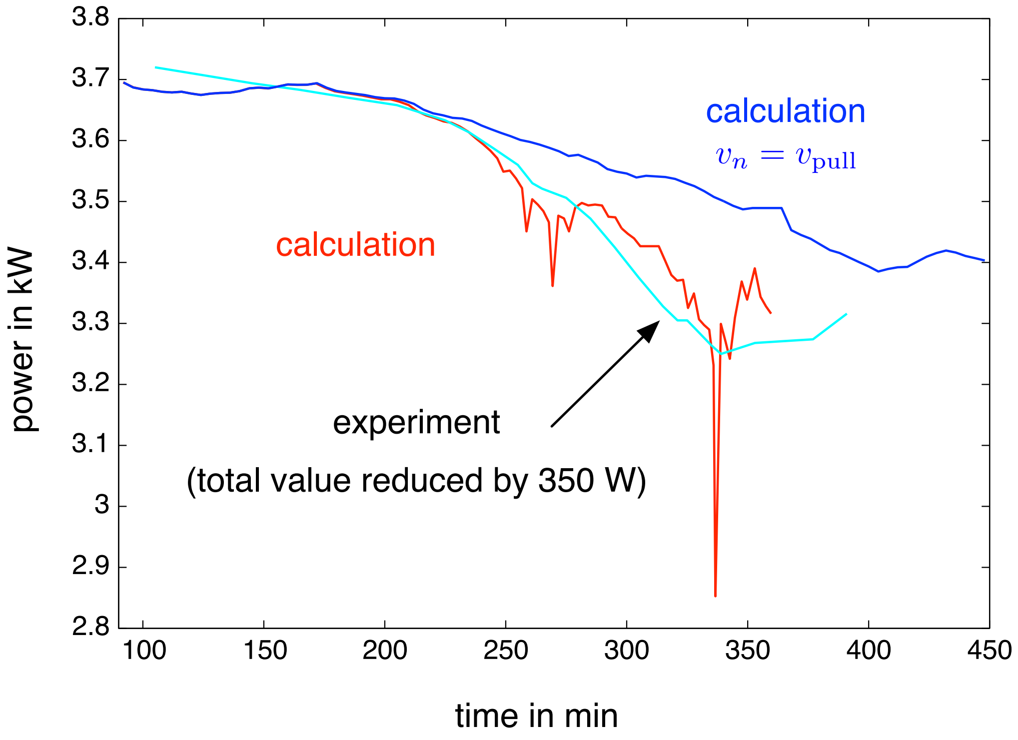
Starting with $\mu = 2 \times 10^{-2}\ \mathrm{Pa\,s}$ and increasing with iteration

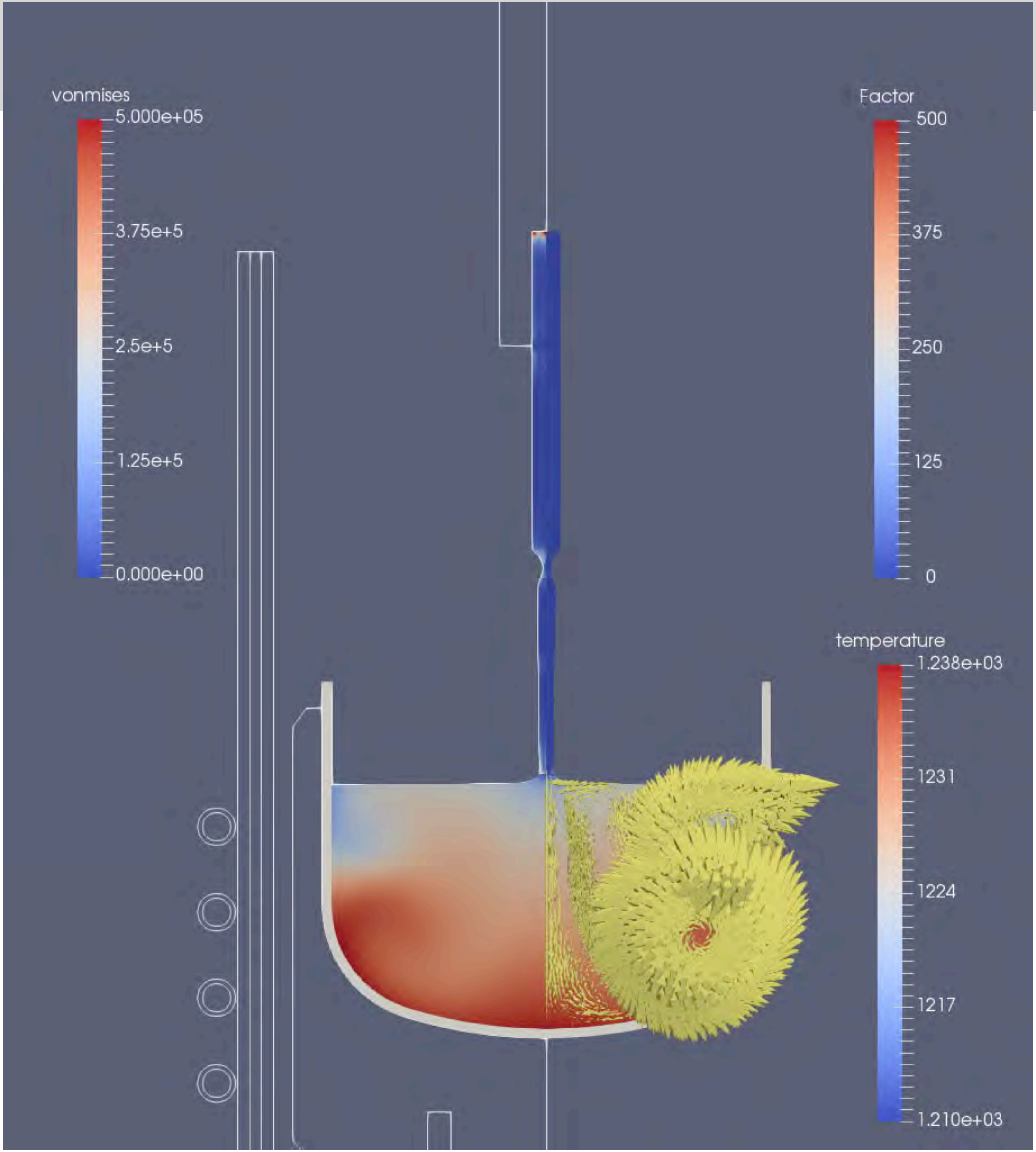
```
Viscosity = Variable Time
  MATC " if ( tx < 20 ) 1.2e-2 - tx/20*7e-3; else 5.0e-3; "
```

Validation

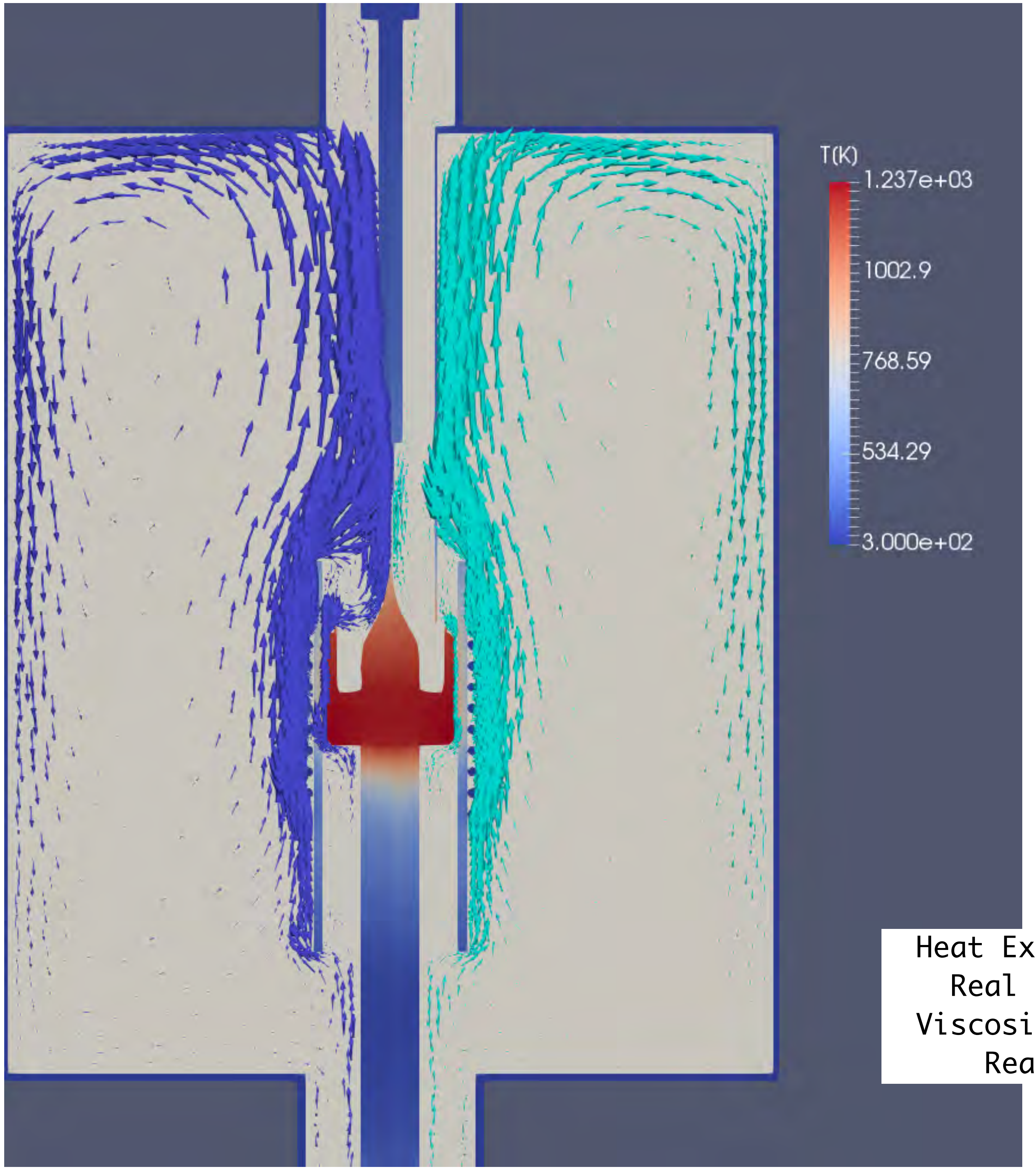


RGZ-69




vonmises
5.000e+05
3.75e+5
2.5e+5
1.25e+5
0.000e+00
Factor
500
375
250
125
0
temperature
1.238e+03
1231
1224
1217
1.210e+03

Gas Convection

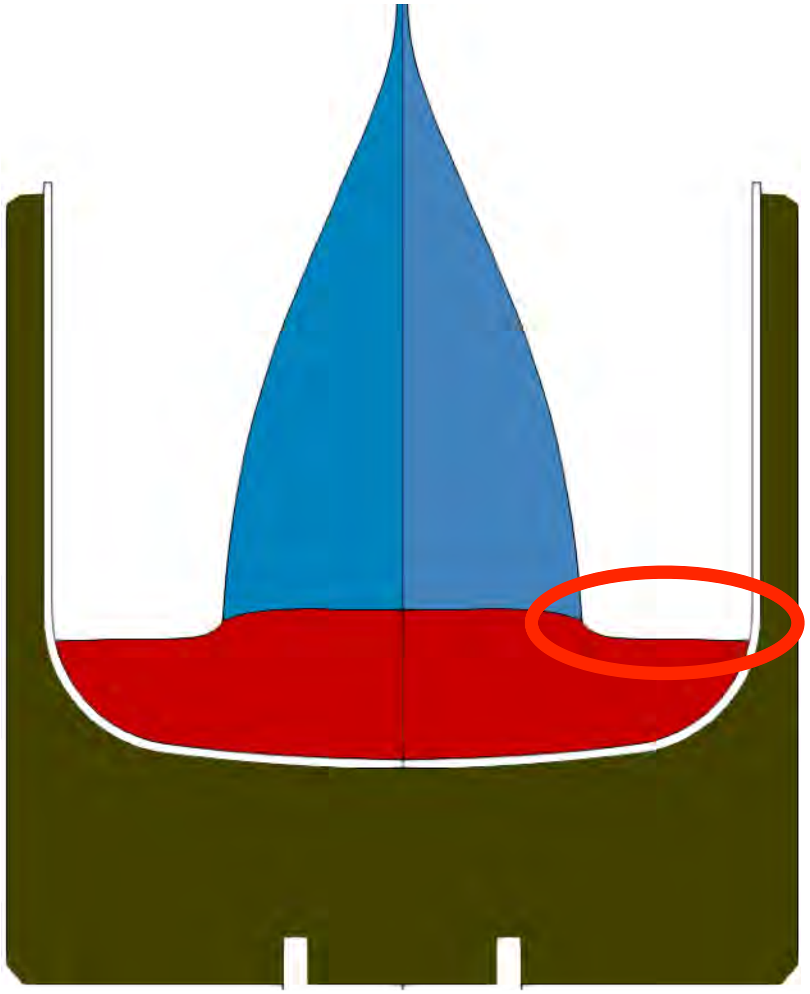


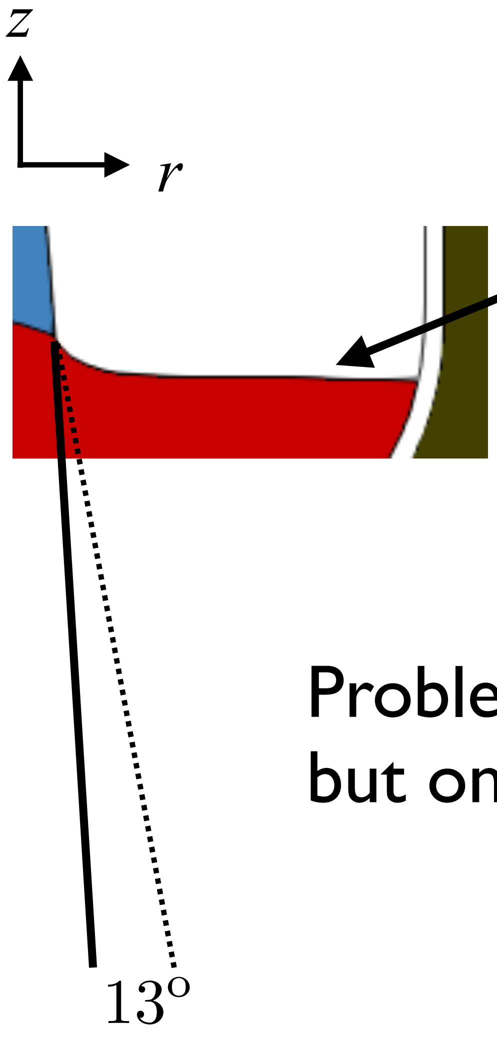
```
Heat Expansion Coefficient = Variable Temperature
  Real MATC " 1.0/tx "
Viscosity =  Variable Temperature
    Real MATC " tx * 3.25e-5 "
```

Current Problems

Computing of melt convection and gas convection:

Solving Navier-Stokes eq. in gas and melt separately





$$u_r^{\mathrm{gas}} \equiv u_r^{\mathrm{melt}}$$

gas

fixed shape

$$\mu \frac{\partial u_r}{\partial z} = \frac{\partial \gamma}{\partial T} \frac{\partial T}{\partial r}$$

melt

Problem: Calling two NS solvers possible but only one velocity field enters Heat Solver

Future Work

- Taking into account change of interface shape into computation of v_n.
  (v_n & latent heat depends on location, $v_n(r)$)

- Computation of dislocation density

- Optimization ?
  Simulation is parameterized
  ⇨ using for optimization strategy over process run ?

Acknowledgements

1	Nikolay Abrosimov	●	head of team
2	Jozsef Janicskó-Csáthy	●	coordinator
2	Jörg Fischer	●	construction & purification
3	Oleksii Gybin	●	crystal growth
4	Stephan Kayser	●	LPS measurements

BMBF-Verbundprojekt GERDA (2017-2020)