pyelmer

Python interface for Elmer workflow

Elmer Webinar series

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Introduction

Arved Enders-Seidlitz, M. Sc.

Engineering Science

PhD Student
„Model development and validation for crystal growth process simulation“

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University of Latvia
Solar World / Uni. Freiberg

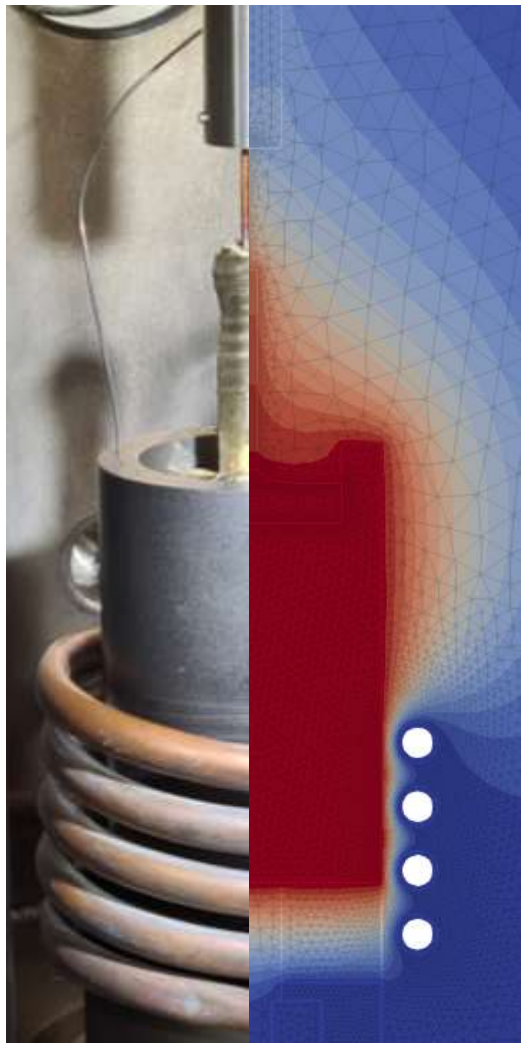
Group Leader „Model Experiments“
NEMOCRYS Project
funded by ERC Starting Grant

Leibniz Institute for Crystal Growth

Germany, Berlin-Adlershof

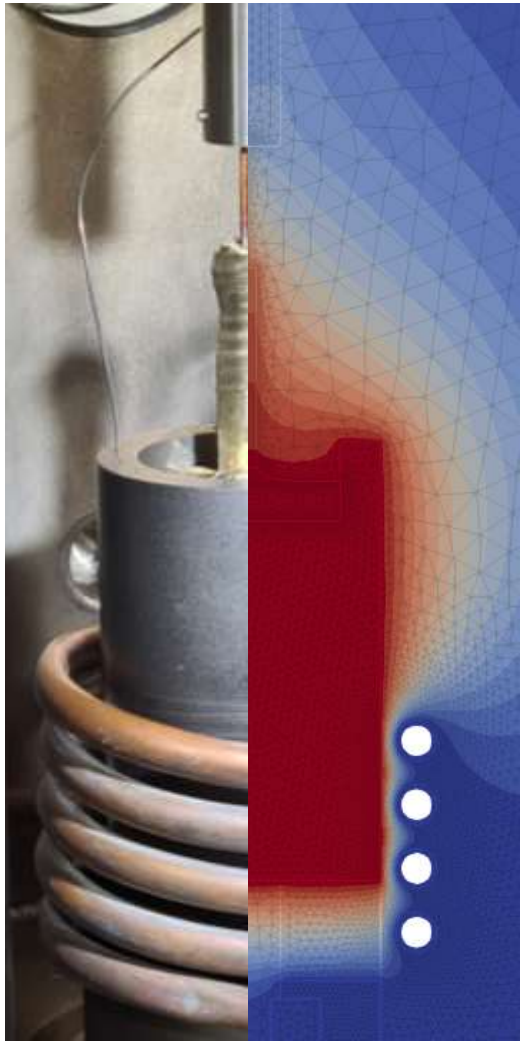
- Fundamental to pre-industrial research
- Development, characterization and production of crystalline materials

Content



- Motivation
- Getting started
- Examples & background
- Application in crystal growth
- Contribution & summary

Content



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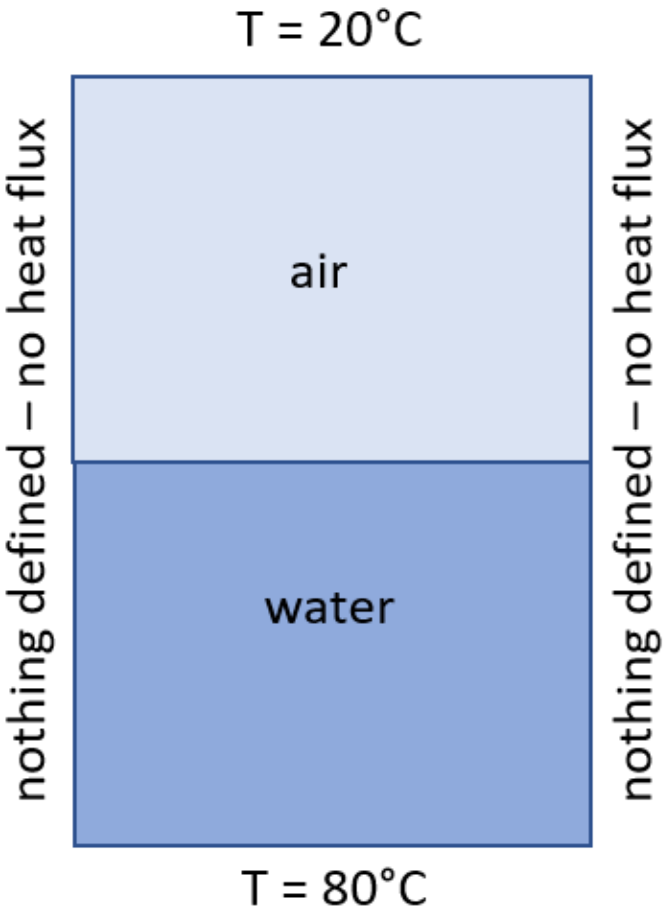
Motivation – the classical workflow

The classical workflow

1. Write *geo*-file, run Gmsh, export mesh
2. Write Elmer *sif*-file
3. Run ElmerGrid, ElmerSolver

Heating up water

- 2D steady state
- Water and air
- Heating at bottom
- Cold top surface
- No heat flux over boundaries
- Only heat conduction *(non-physical!)*



Motivation – the classical workflow

1. **Write *geo*-file, run Gmsh, export mesh**
2. Write Elmer *sif*-file
3. Run ElmerGrid, ElmerSolver

Workflow

- Create points, …
- … lines from points, …
- … loops from lines, …
- … surfaces from loops, …
- … and physical groups.

- Complex numbering required

```
Point(1) = {0, 0, 0};
Point(2) = {1, 0, 0};
Point(3) = {1, 1, 0};
Point(4) = {0, 1, 0};
Point(5) = {1, 2, 0};
Point(6) = {0, 2, 0};

Line(1) = {1, 2};
Line(2) = {2, 3};
Line(3) = {3, 4};
Line(4) = {4, 1};
Line Loop(101) =  {1, 2, 3, 4};
Plane Surface(101) = {101};

Line(5) = {5, 3};
Line(6) = {6, 5};
Line(7) = {4, 6};
Line Loop(102) = {7, 6, 5, 3};
Plane Surface(102) = {102};

Physical Surface ("Water") = {101};
Physical Surface ("Air") = {102};

Physical Line ("Bottom") = {1};
Physical Line ("Top") = {6};

Mesh(2);
Save "mesh.msh";
```

Motivation – the classical workflow

1. Write *geo*-file, run Gmsh, export mesh
2. **Write Elmer *sif*-file**
3. Run ElmerGrid, ElmerSolver

Workflow

- Copy setup from Elmer test cases
- Adapt solver parameter as far as you understand them
- Insert bodies, materials, boundaries
- Set relations by IDs

```
Header
  CHECK KEYWORDS "Warn"
  Mesh DB "." "."
End

Simulation
  Max Output Level = 4
  Coordinate System = Cartesian 2D
  Simulation Type = Steady state
  Steady State Max Iterations = 10
End

Equation 1
  Active Solvers(1) = 1
End

Solver 1
  Equation = HeatSolver
  Procedure = "HeatSolve" "HeatSolver"
  Variable = "Temperature"
  Variable Dofs = 1
  Calculate Loads = True
  Exec Solver = Always
  Nonlinear System Convergence Tolerance = 1e-06
  Nonlinear System Max Iterations = 1000
  Nonlinear System Relaxation Factor = 0.7
  Steady State Convergence Tolerance = 1e-06
  Stabilize = True
  Optimize Bandwidth = True
  Linear System Solver = Iterative
  Linear System Iterative Method = BiCGStab
  Linear System Max Iterations = 1000
  Linear System Preconditioning = ILU
  Linear System Precondition Recompute = 1
  Linear System Convergence Tolerance = 1e-08
  Linear System Abort Not Converged = True
  Linear System Residual Output = 1
End

Solver 2
  Exec Solver = After timestep
  Equation = ResultOutputSolver
  Procedure = "ResultOutputSolve" "ResultOutputSolver"
  VTU Format = True
  Save Geometry Ids = Logical True
End
```

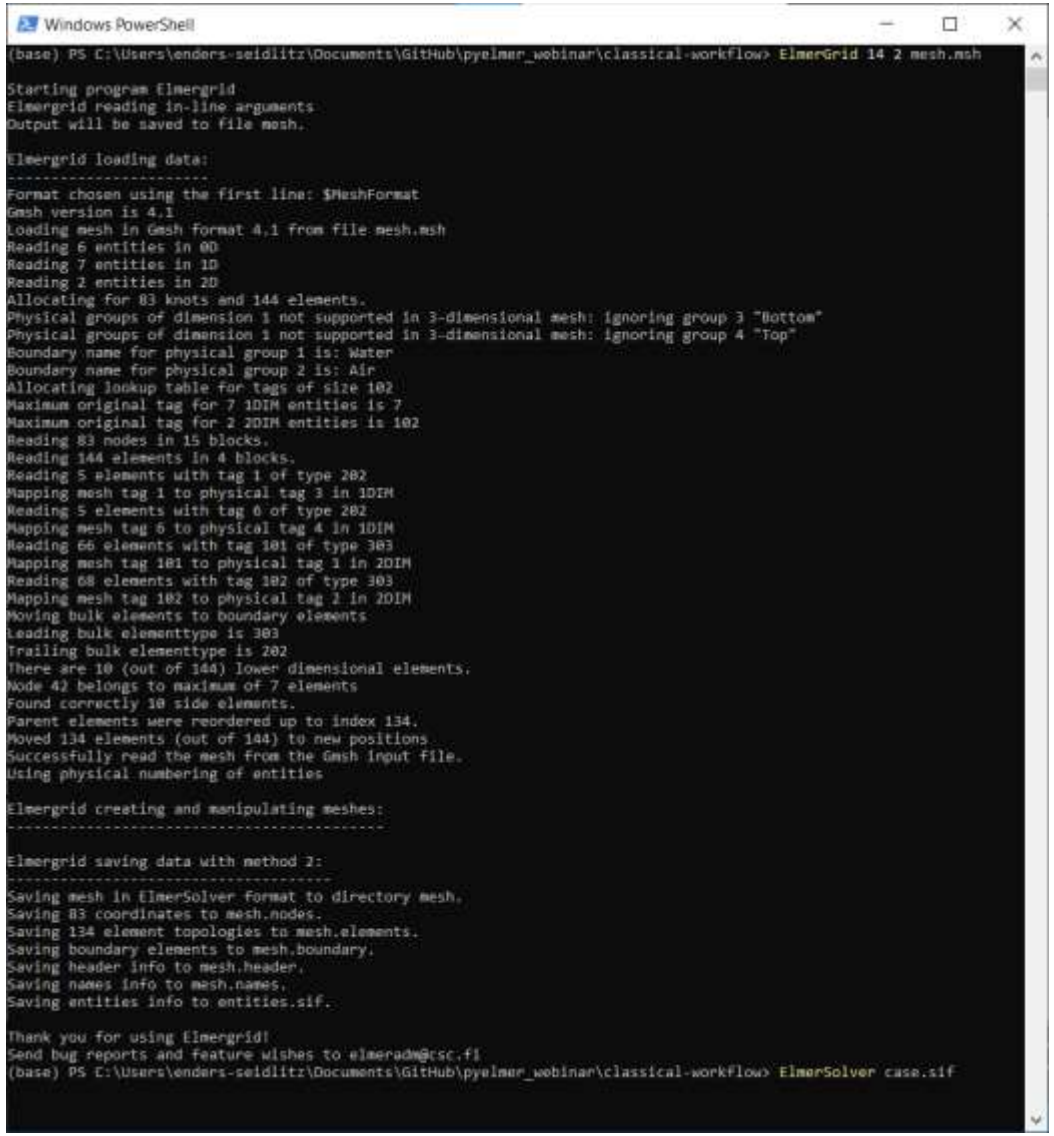
```
Material 1
  Density = 1.1885
  Heat Capacity = 1006.4
  Heat Conductivity = 0.025873
End

! water
Material 2
  Density = 1000.0
  Heat Capacity = 4182.0
  Heat Conductivity = 0.6
End

Body 1
  Target Bodies(1) = 1
  Equation = 1  ! main
  Initial Condition = 1  ! T0
  Material = 2  ! water
End

Body 2
  Target Bodies(1) = 2
  Equation = 1  ! main
  Initial Condition = 1  ! T0
  Material = 1  ! air
End

Boundary Condition 1
  Target Boundaries(1) = 3
  Temperature = 353.15
End

Boundary Condition 2
  Target Boundaries(1) = 4
  Temperature = 293.15
End

Initial Condition 1
  Temperature = 273.15
End
```

Motivation – the classical workflow

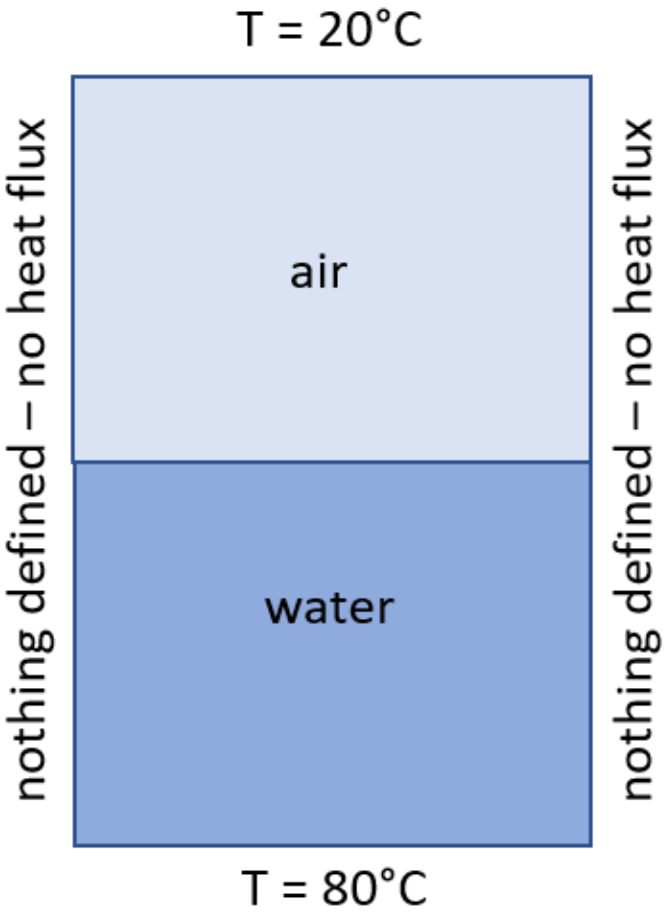
1. Write *geo*-file, run Gmsh, export mesh
2. Write Elmer *sif*-file
3. **Run ElmerGrid, ElmerSolver**

Workflow

- Open shell
- Execute ElmerGrid
- Execute ElmerSolver
- (Read solver output)



Motivation – the classical workflow



Conclusion

- Hard to understand
- Easy to make mistakes
- Difficult to debug

- Too much manual work
- Too many IDs

Motivation – the pyelmer workflow

Create clean code…

Keep it simple, stupid (KISS)

- Everything in one place
  - Geometry, mesh
  - Simulation setup, control
- Easy to read, write and understand

Do not repeat yourself (DRY)

- Default parameters stored separately
  - Solvers, Materials
- Re-usable by modular design

…for beginners and experts

Programming language: Python

- Most popular
- Infrastructure and feature set
- **…**

Open parameter space

- Default solvers for beginners
- Customizable for experts

Motivation – the pyelmer workflow

```python
import os, gmsh, pyelmer

sim_dir = "./simdata"
if not os.path.exists(sim_dir):
    os.mkdir(sim_dir)

gmsh.initialize()
gmsh.option.setNumber("General.Terminal", 1)
gmsh.model.add("heat-transfer-2d")
factory = gmsh.model.occ

water = factory.addRectangle(0, 0, 0, 1, 1)
air = factory.addRectangle(0, 1, 0, 1, 1)
factory.synchronize()
factory.fragment([(2, water)], [(2, air)])
factory.synchronize()
ph_water = pyelmer.gmsh.add_physical_group(2, [water], "water")
ph_air = pyelmer.gmsh.add_physical_group(2, [air], "air")

line = pyelmer.gmsh.get_boundaries_in_box(0, 0, 0, 1, 0, 0, 2, water)
ph_bottom = pyelmer.gmsh.add_physical_group(1, [line], "bottom")
line = pyelmer.gmsh.get_boundaries_in_box(0, 2, 0, 1, 2, 0, 2, air)
ph_top = pyelmer.gmsh.add_physical_group(1, [line], "top")

gmsh.model.mesh.setSize(gmsh.model.getEntities(0), 0.1)
gmsh.model.mesh.generate(2)
gmsh.write(sim_dir + "/case.msh")

sim = pyelmer.elmer.load_simulation("2D_steady")
air = pyelmer.elmer.load_material("air", sim)
water = pyelmer.elmer.load_material("water", sim)
solver_heat = pyelmer.elmer.load_solver("HeatSolver", sim)
solver_output = pyelmer.elmer.load_solver("ResultOutputSolver", sim)
eqn = pyelmer.elmer.Equation(sim, "main", [solver_heat])
T0 = pyelmer.elmer.InitialCondition(sim, "T0", {"Temperature": 273.15})

bdy_water = pyelmer.elmer.Body(sim, "water", [ph_water])
bdy_water.material = water
bdy_water.initial_condition = T0
bdy_water.equation = eqn

bdy_air = pyelmer.elmer.Body(sim, "air", [ph_air])
bdy_air.material = air
bdy_air.initial_condition = T0
bdy_air.equation = eqn

bndry_bottom = pyelmer.elmer.Boundary(sim, "bottom", [ph_bottom])
bndry_bottom.fixed_temperature = 353.15  # 80 °C
bndry_top = pyelmer.elmer.Boundary(sim, "top", [ph_top])
bndry_top.fixed_temperature = 293.15  # 20 °C

sim.write_startinfo(sim_dir)
sim.write_sif(sim_dir)

pyelmer.execute.run_elmer_grid(sim_dir, "case.msh2")
pyelmer.execute.run_elmer_solver(sim_dir)

err, warn, stats = pyelmer.post.scan_logfile(sim_dir)
print(„\nErrors:", err, „\nWarnings:", warn, „\nStatistics:", stats)
```

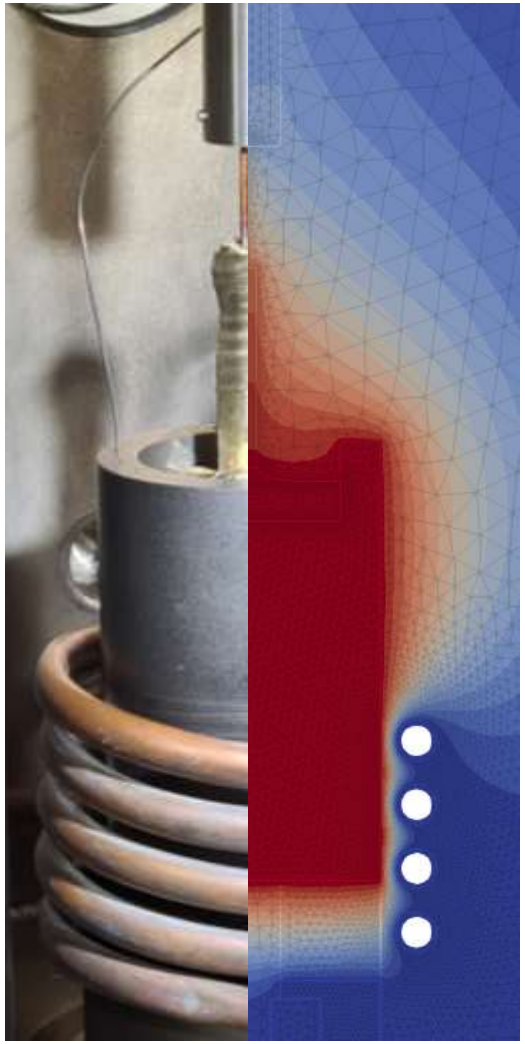
pyelmer

- Gmsh python API
- Object-oriented relation management
- Execute & evaluate

- 50 lines of code for “heating up water” case

  (geo-file: 23 lines, sif-file: 74 lines)

Content



Motivation

Getting started

Examples & background

Application in crystal growth

Contribution & summary

Getting started with pyelmer

Where to find it

- https://github.com/nemocrys/pyelmer
- https://pypi.org/project/pyelmer/

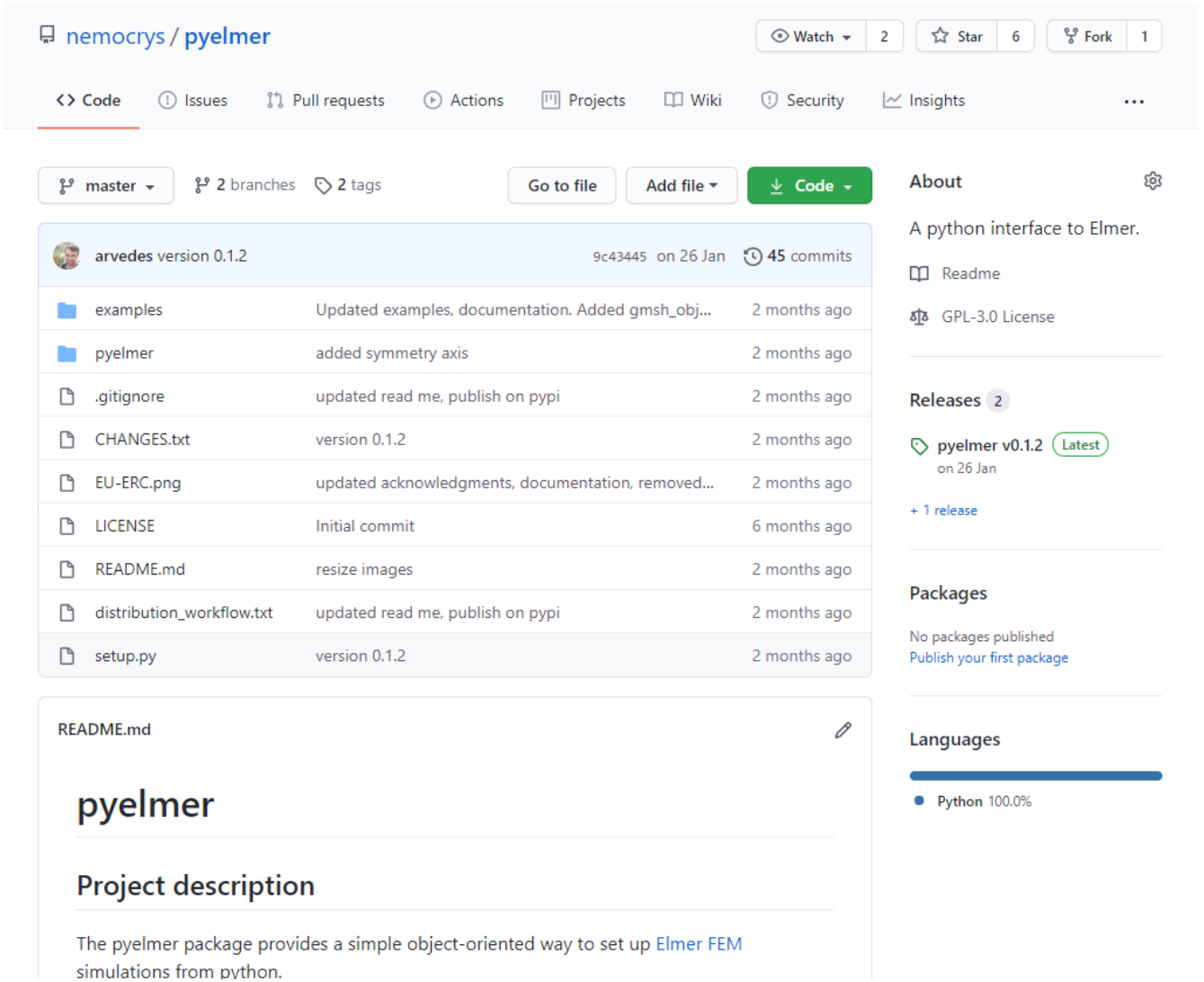
How to install it

- `pip install pyemer`
- ElmerSolver, ElmerGrid executable on path

What to do with it

- Examples in readme on Github
- Or in examples folder
- Docstrings in source code

License: GPL v3



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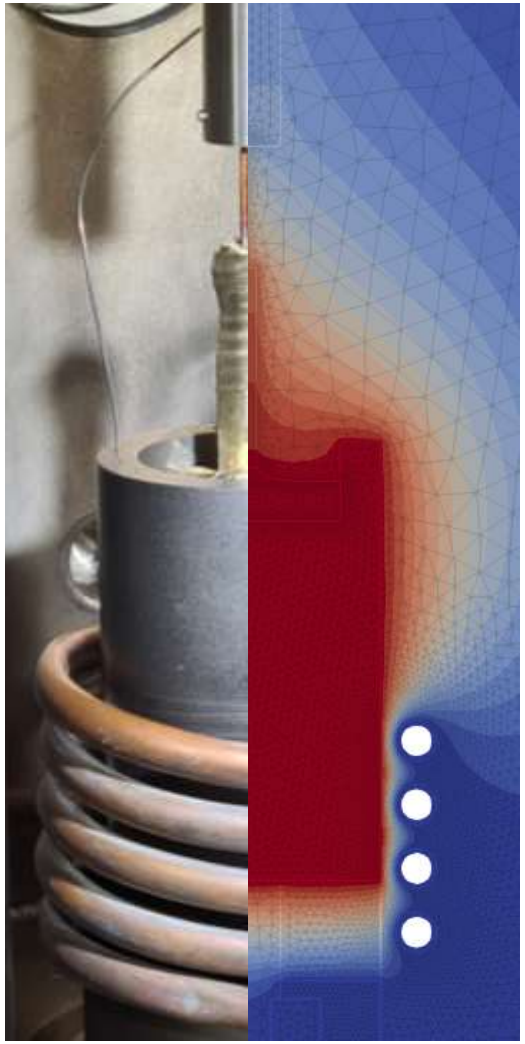

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Example 1 – heating up water

https://youtu.be/KZ1N2FM6J7E

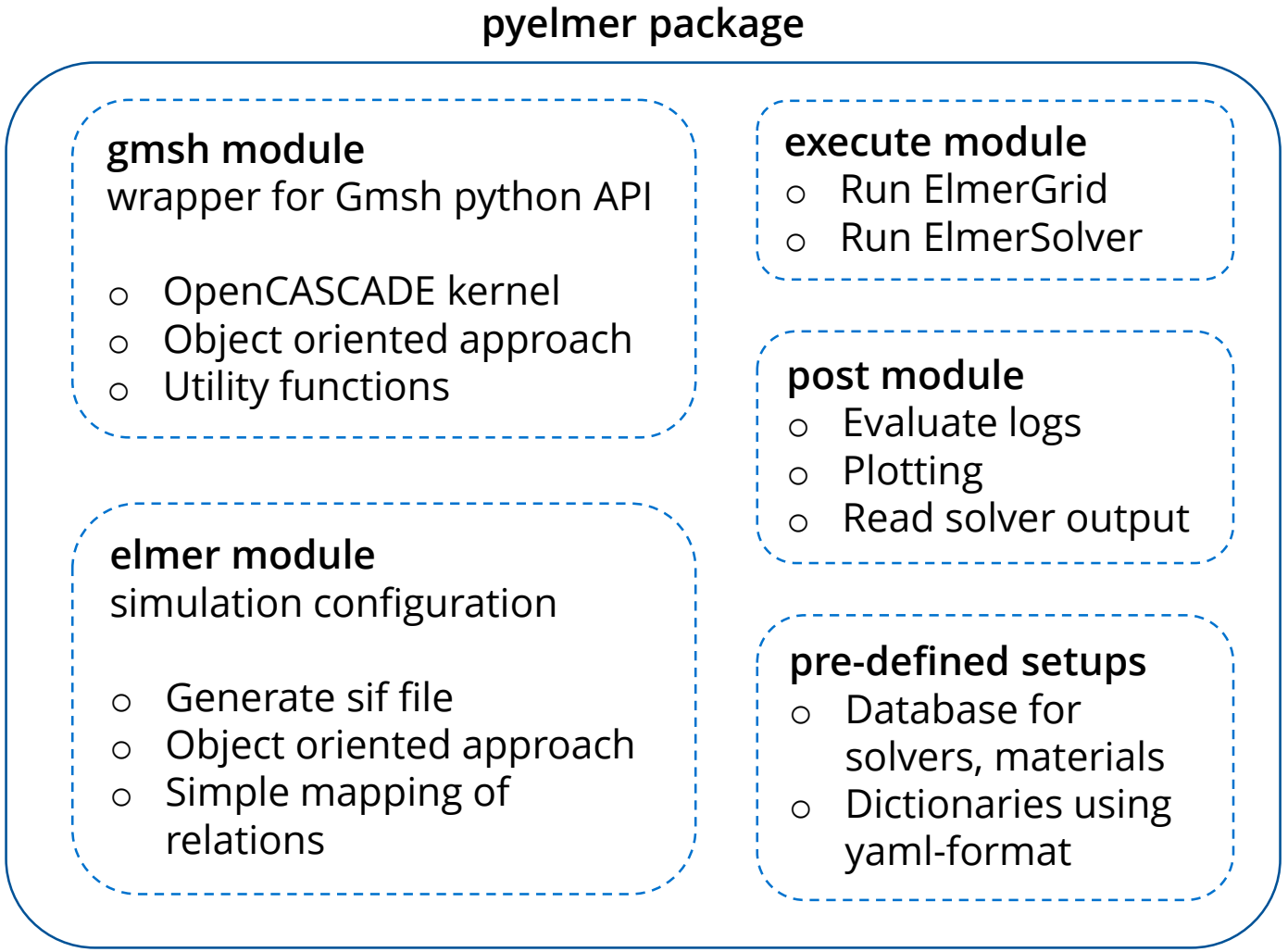
Background – design of pyelmer

Focused on workflow

- Mesh generation in Python using Gmsh
- Setup with in Python
- Simulation with ElmerSolver
- Postprocessing with paraview, pyelmer, custom python scripts

Design considerations

- Follow Elmer defined structure (sif file)
- Provide open keyword space
- Fully automatize the annoying stuff



Example 2 – crystal growth

https://youtu.be/0lnX-ytKTH8

Background – gmsh module

pyelmer package

gmsh module
wrapper for Gmsh python API

- OpenCASCADE kernel
- Object oriented approach
- Utility functions

execute module
- Run ElmerGrid
- Run ElmerSolver

post module
- Evaluate logs
- Plotting
- Read solver output

elmer module
simulation configuration

- Generate sif file
- Object oriented approach
- Simple mapping of relations

pre-defined setups
- Database for solvers, materials
- Dictionaries using yaml-format

Mesh generation with gmsh

- gmsh python API
  - Native way to use it
  - Complex and cumbersome
- pyelmer.gmsh
  - Object-oriented top-to-bottom approach (with OpenCASADE kernel)
  - Utility functions for gmsh python API
- pygmsh
  - Independent gmsh interface
  - Improved workflow

Background – gmsh module

Classes for geometry modeling and mesh generation

`class Model`

- Collect geometries (Shape objects)
- Generate and export mesh
- Global Gmsh operations

`class Shape`

- Wrapper for any kind of shape:

  Bodies, surfaces, lines, …
- Defined by Gmsh geometry ID
- Simplifies Gmsh operations: Extract boundaries

Classes for mesh control

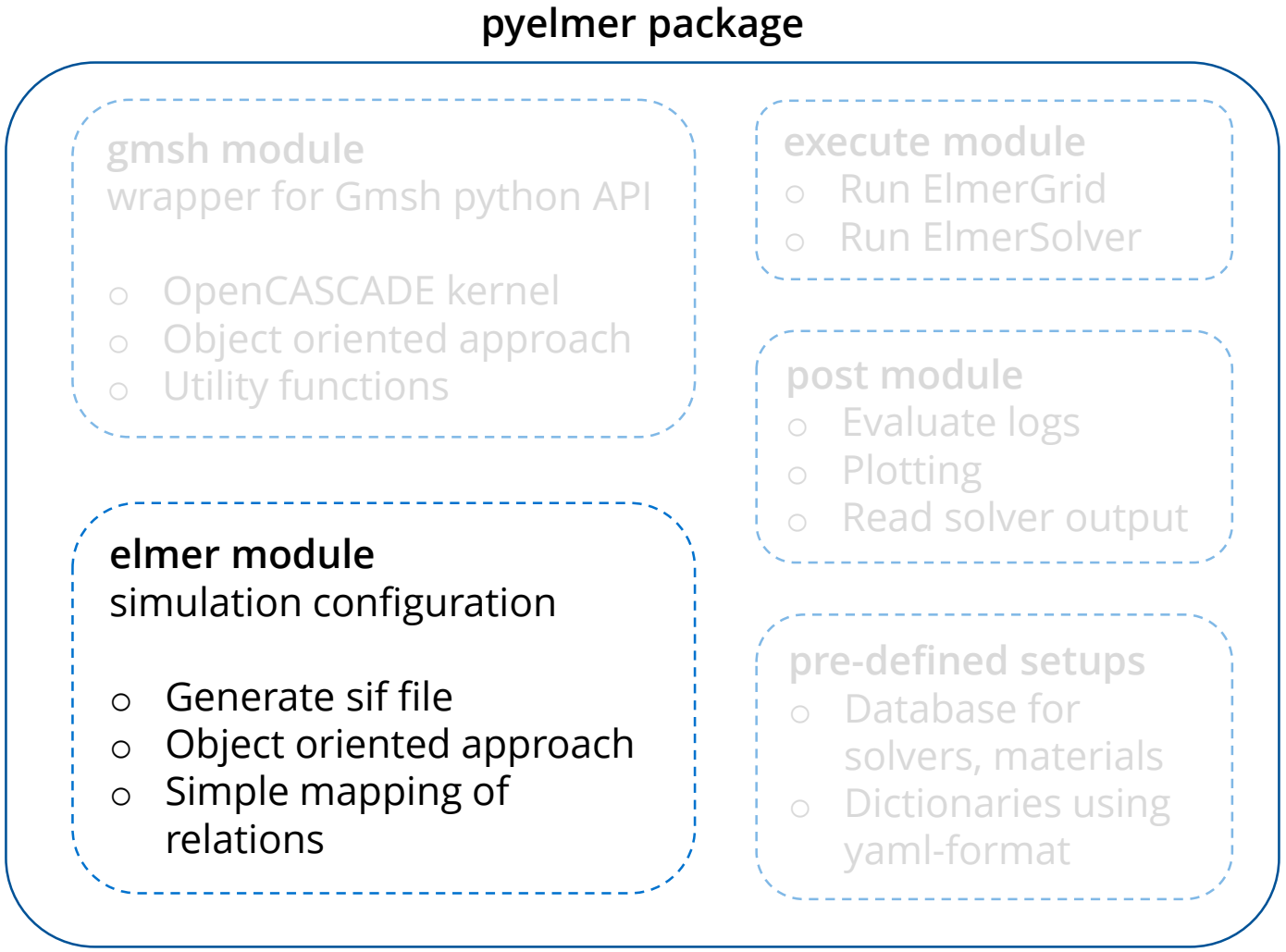
- `class MeshControlConstant`
- `class MeshControlLinear`
- `class MeshControlExponential`

Working principle

- Wrapper for Gmsh API
- In case of errors: plot the model

```
model.synchronize()
model.show()
```

Background – elmer module



`class Simulation`

- Global settings
- Sub-components
- Writes sif-file

Classes for sub-compontens

`Solver, Equation, Material, Body, BodyForce, InitialCondition, Boundary`

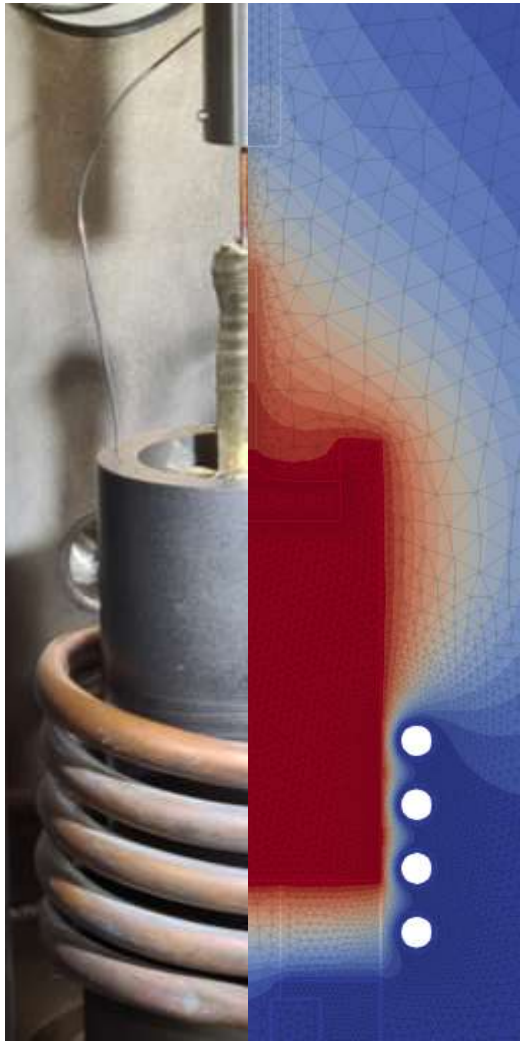
Functions to load setups

`Simulation, Solver, Material`

Background – elmer module

Let’s have a look at the code!

Content



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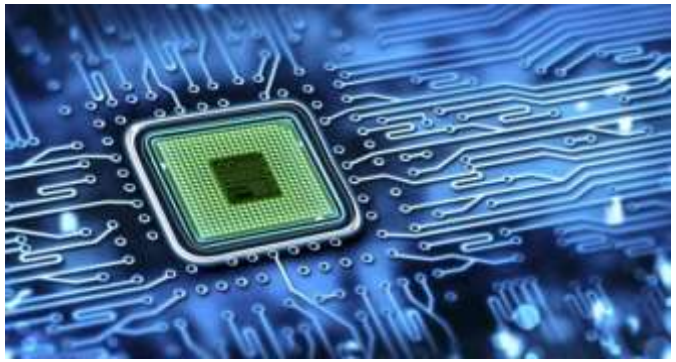


http://www.knoda.org/back-history-discovery-very-first-silicon-chip-digital-computers/

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

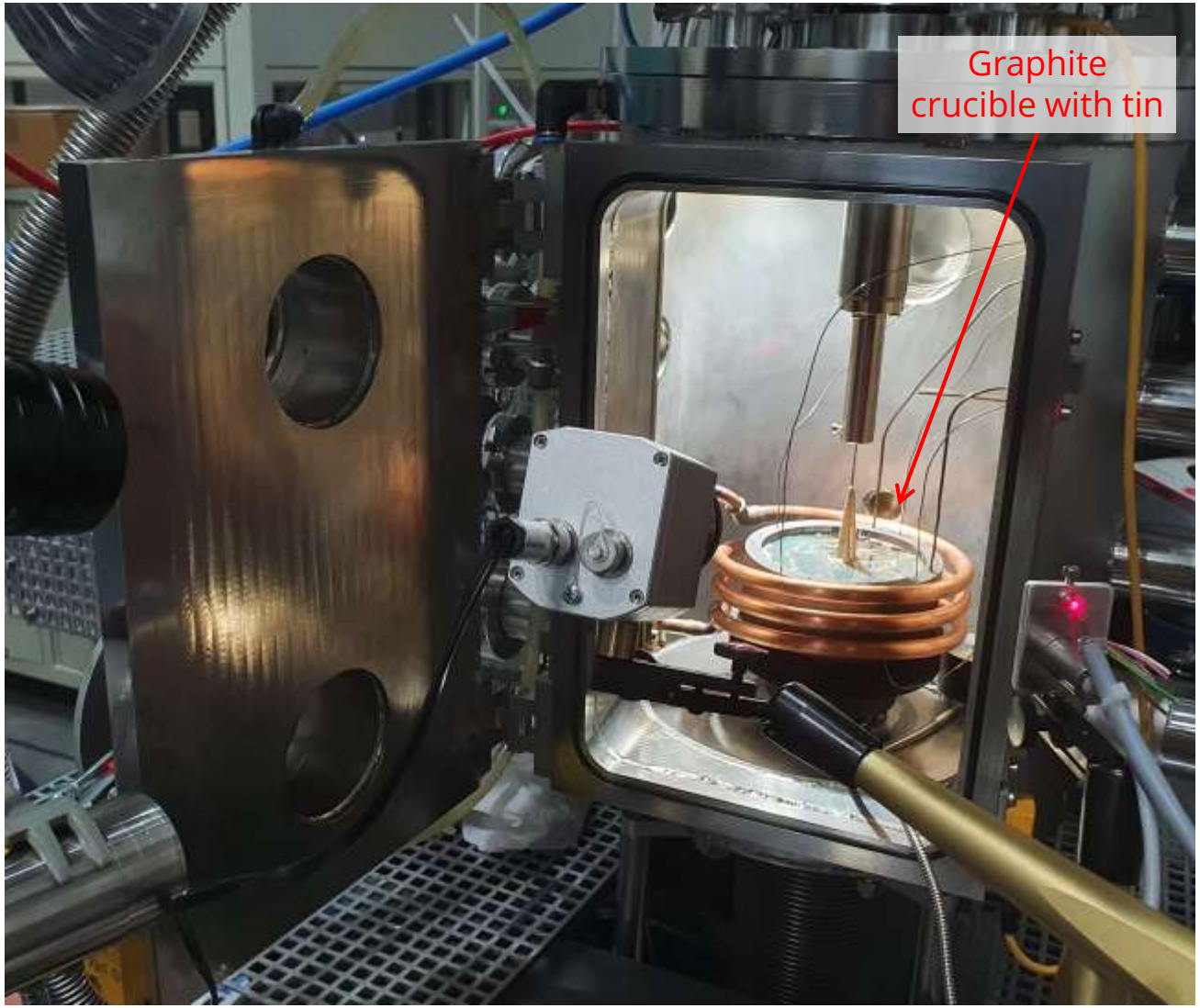
Silicon single crystal

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

Silicon growth furnace

Application in crystal growth

NEMOCRYS: Next Generation Multiphysical Models for Crystal Growth Processes



Model materials

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

Conditions

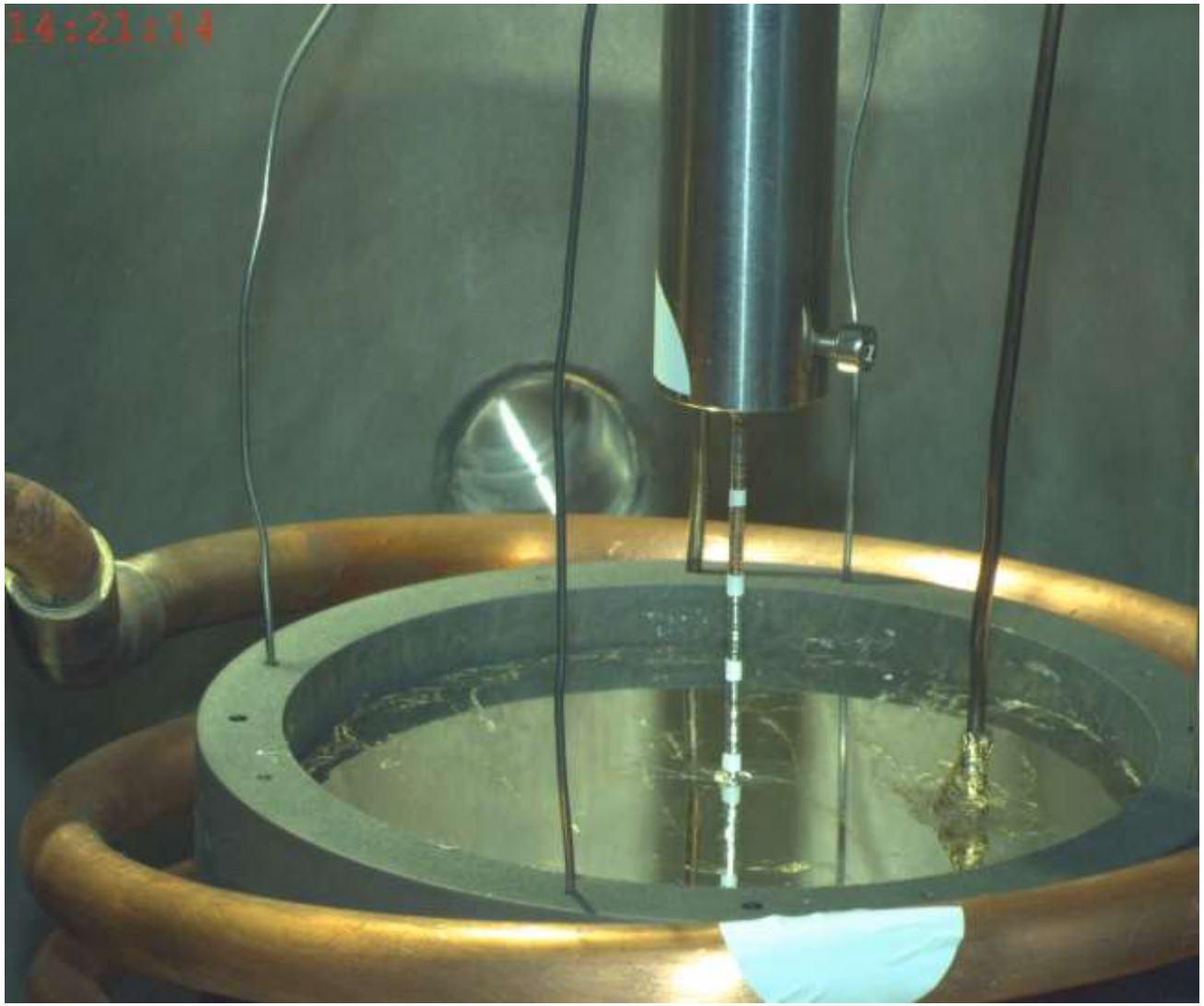
- Air atmosphere (cooling with fan)
- Vacuum

Measurements

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

Application in crystal growth

NEMOCRYS: Next Generation Multiphysical Models for Crystal Growth Processes



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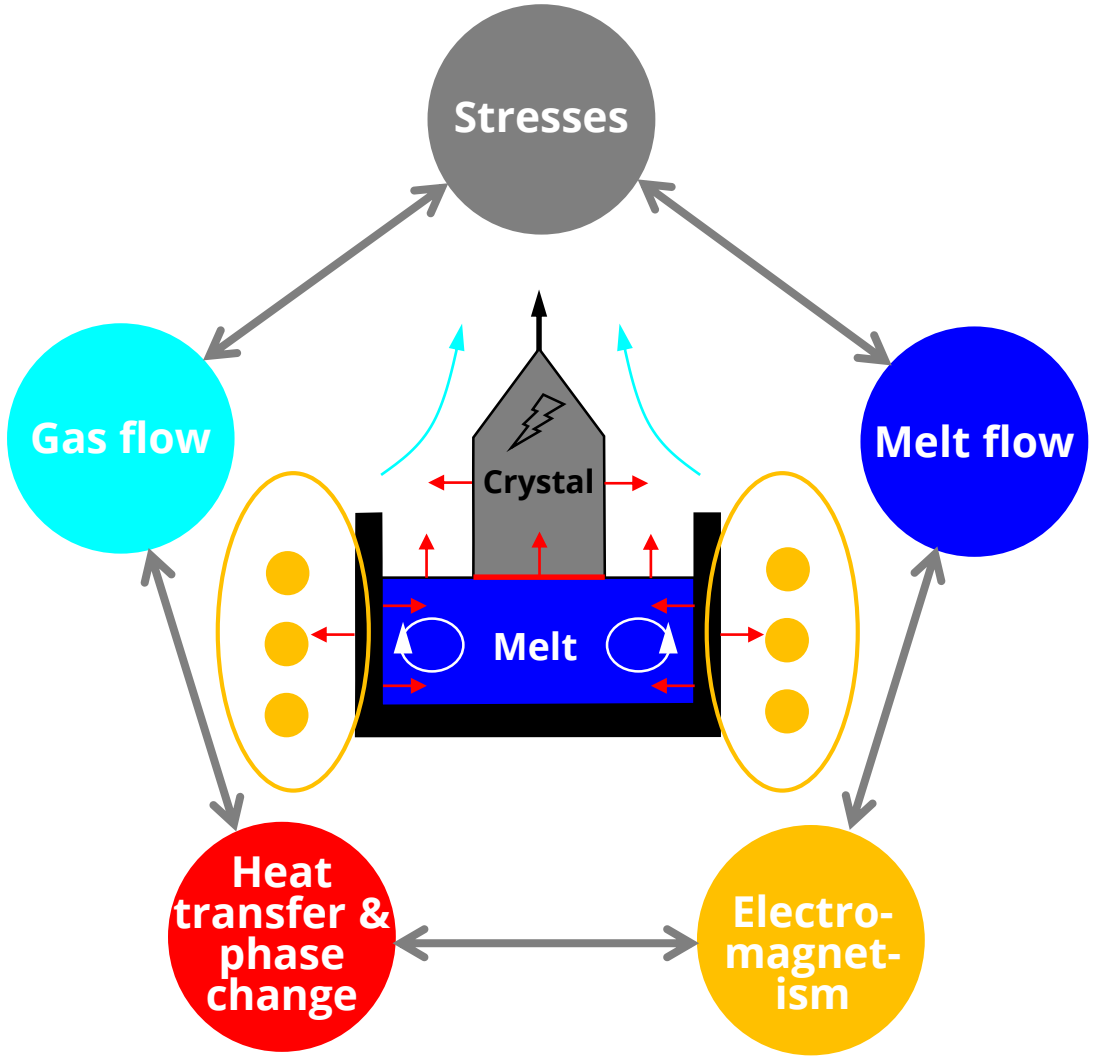
Application in crystal growth



Numerical challenges

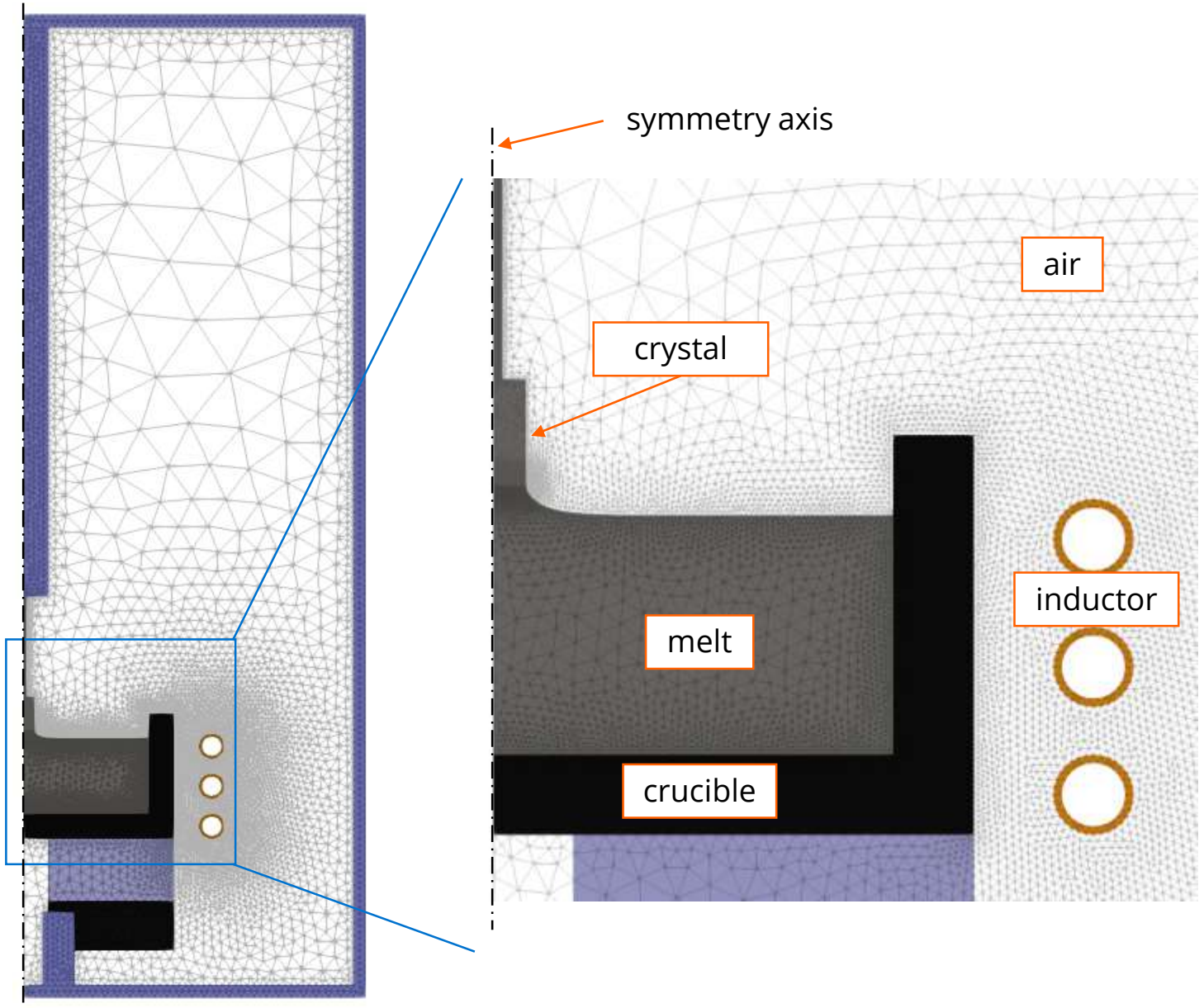
- Complex coupled physics
- Moving geometries
- Heat radiation
- …

Goals in NEMOCRYS Project

- Validation: Using model experiments
- Open source implementation

→ Elmer provides the best feature set

Application in crystal growth



Induction heating (2D axisymmetric, 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 (2D axisymmetric)

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

Phase change (2D axisymmetric, steady-state)

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

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/

Application in crystal growth

Procedure using Elmer / Gmsh

Steady state simulation

↓ T ↓

Mesh generation (with new L)

↓

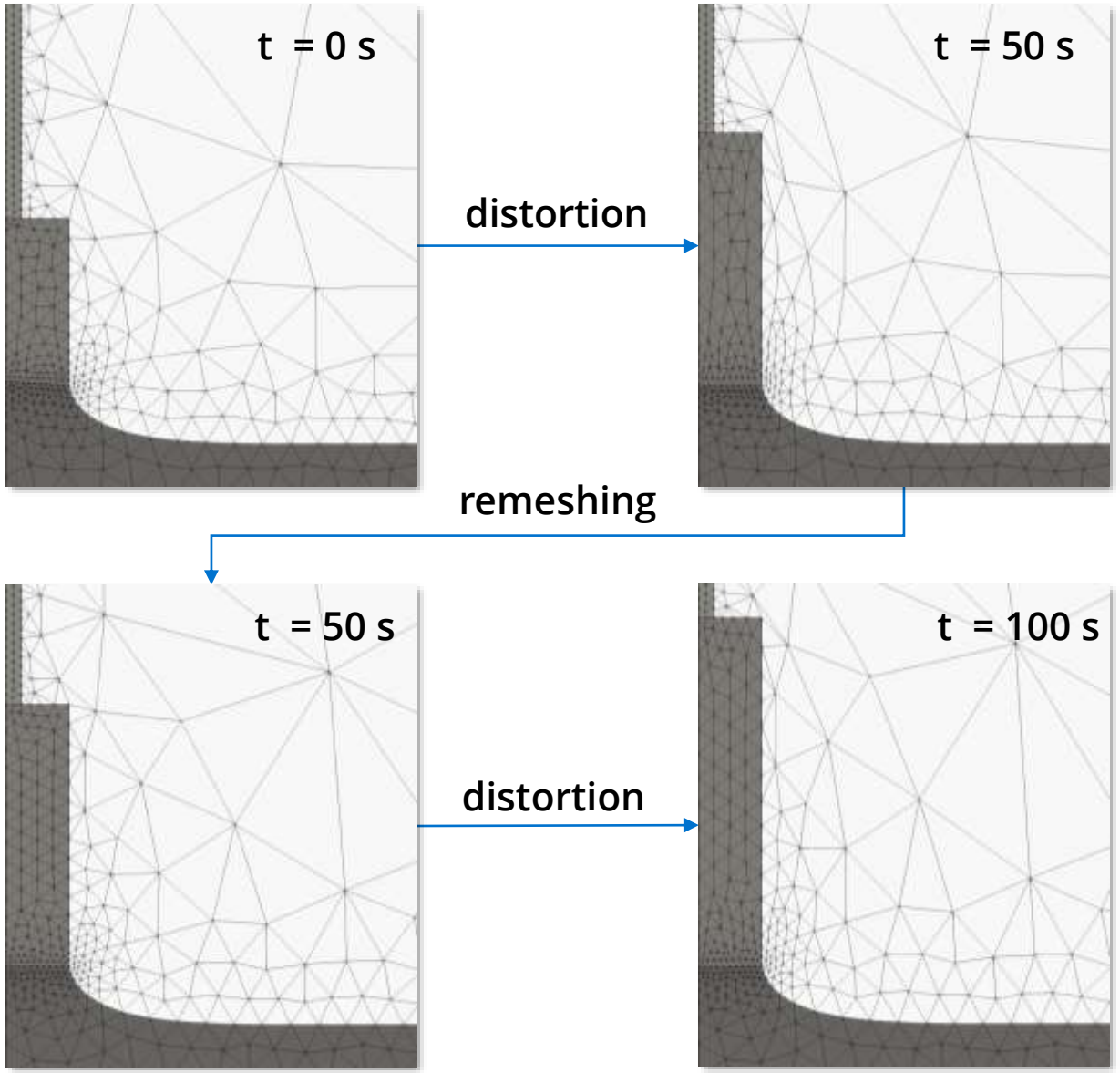
Mesh to mesh interpolation in Elmer

↓

Transient simulation
with mesh distortion

if $l_{crstal} < l_{max}$ | L, T ↓ *else*

Combination of sub-simulations to
one final result in Python



Application in crystal growth

Complex Elmer setup

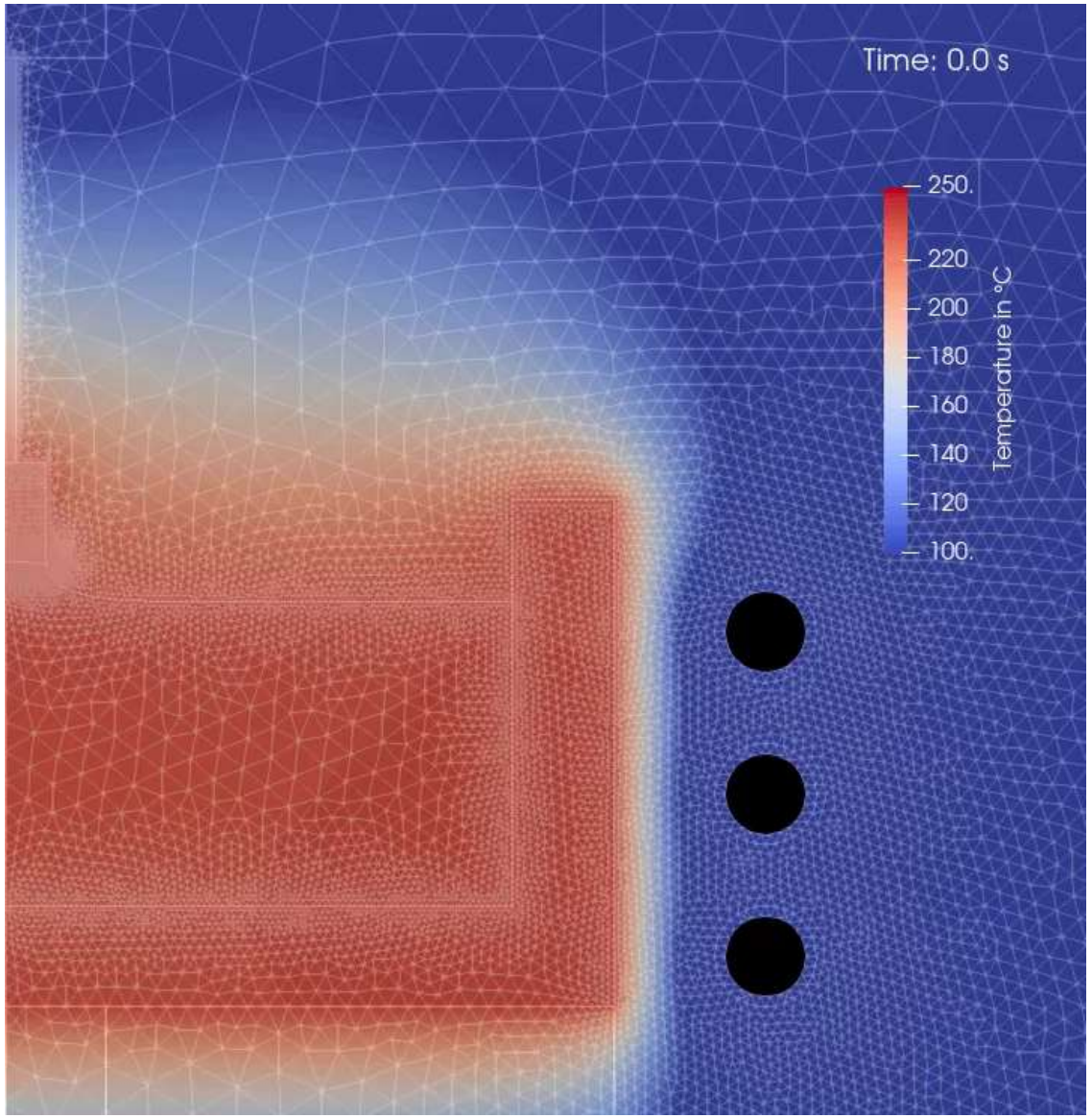
- 9 different solvers, e.g.
  - StatMagSolver / MagnetoDynamics2DHarmonic
  - HeatSolver
  - SteadyPhaseChange
- 12 bodies
- 25 boundary conditions

Combination of different simulation

- Initial steady state simulation
- Series of transient simulations with mesh update

Parameter studies

- Material parameters: 35
- Shape parameters: 30
- Numerical parameters, e.g. mesh, convergence criteria



https://youtu.be/bM0DapM4Ngk

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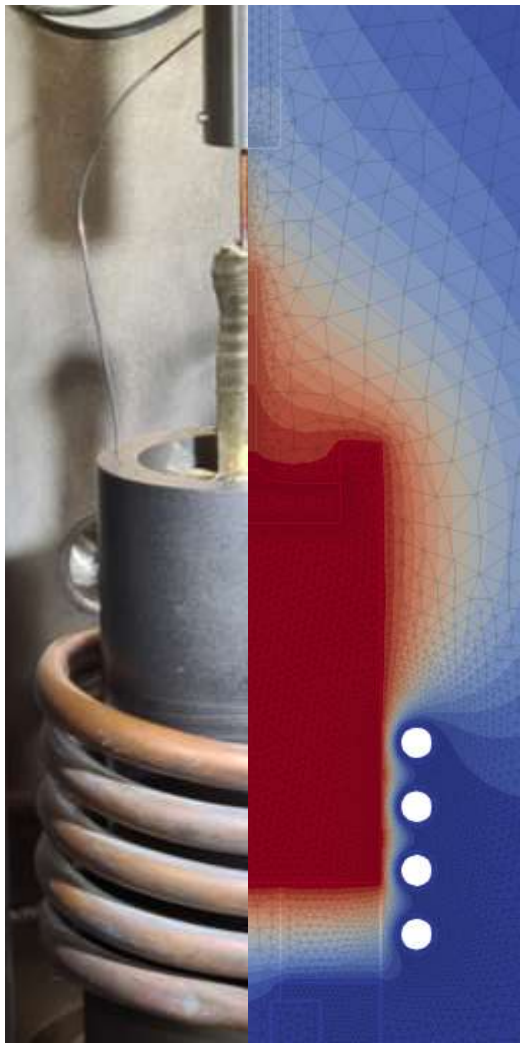

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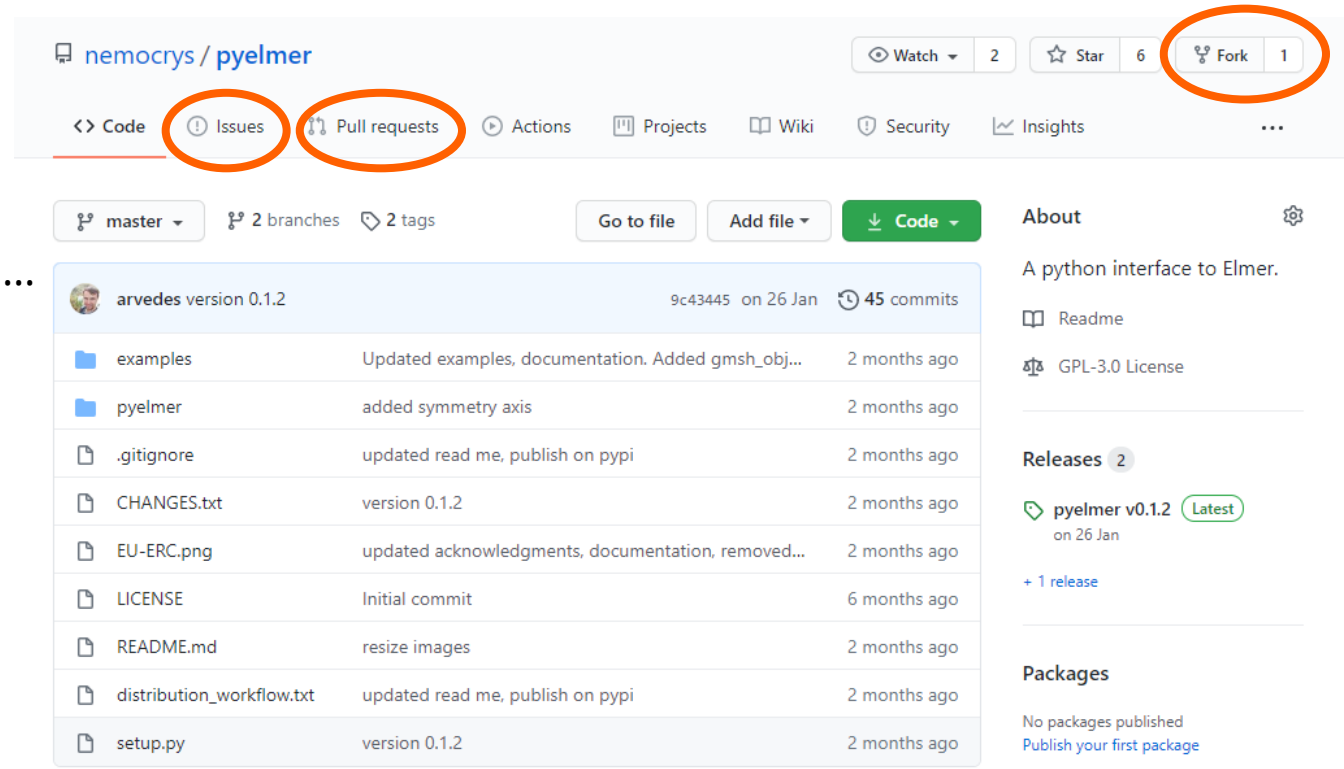
Contribution & summary

Contribution

Open points in the pyelmer development

- Testing
- Documentation – conforming with Elmer docs
- New parameters for bodies, boundary conditions, …
- Add solvers, materials in yaml database
- Consistency checks (for sif file)
- MPI support
- Post processing
  - Evaluation of logs
  - Plot residuals
  - Read output to useful python data format (pandas?)
- # TODO in code
- Additional ideas welcome!



Use github: https://github.com/nemocrys/pyelmer

- Open issue for bugs / feature requests
- Create fork fork / pull request for contribution

Summary

Python workflow for Elmer

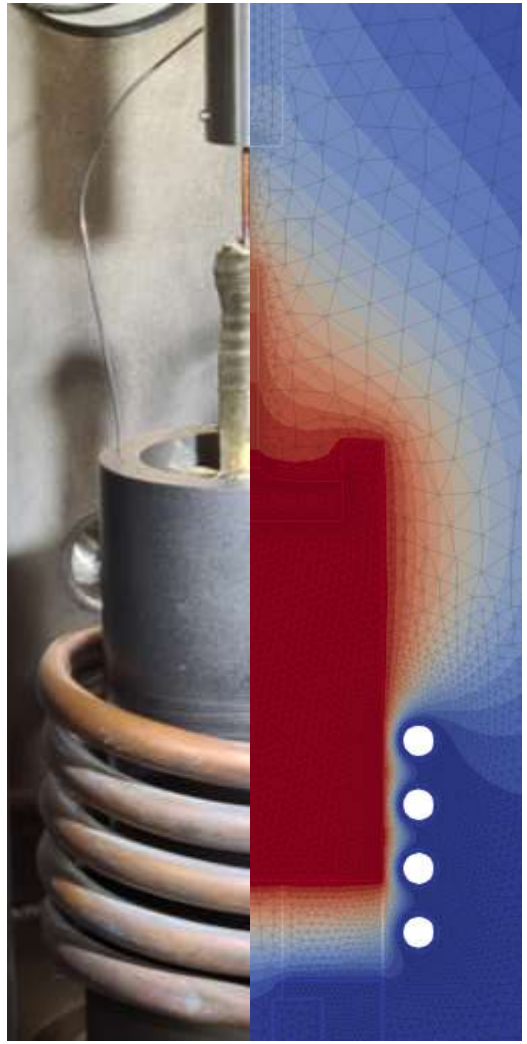
- Geometry & meshing with Gmsh
- Object oriented setup of Elmer

Different examples

- Easy to use for beginners
- High flexibility for all kinds of simulation
- Applied in complex crystal growth simulation

Support us

- Cite pyelmer: https://doi.org/10.5281/zenodo.4431440
- Give us a star on Github
- Provide feedback
- NEMOCRYS Project on ResearchGate



Acknowledgements

Thank you for your attention!

We'd like to acknowledge the developers of Elmer and Gmsh for creating such great open-source software.
Special thanks go to Peter Råback for his support regarding the usage of Elmer.

We'd like to thank Anil Kunwar for his contribution to pyelmer.

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