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Formulations, Software Toolchain and Parallel Methods for FiQuS

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Special thanks to all collaborators, especially from ULiège, the STEAM Team and TU Darmstadt

TE-MPE-PE Section Meeting, CERN, June 26, 2024

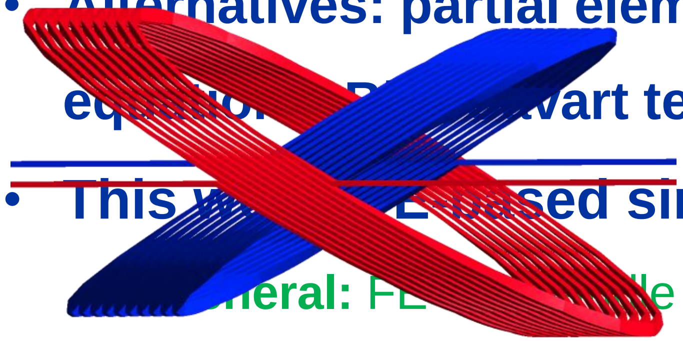
Outline of the Talk

- **Why Finite Elements?**
- **Brief Introduction to FiQuS**
  - CERNGetDP Computing Environment
- **Two FiQuS Models in Detail**
  - Thin Shell Approximations
  - FiQuS-Multipole
  - FiQuS-Pancake3D
- **Early Parallelization in FiQuS**
  - Parallelization in time and space.
- **Conclusion and Outlook**

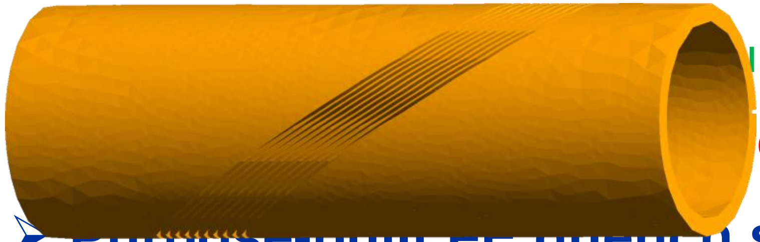
Please feel free to interrupt and ask questions right away!

Why Finite Elements (FE)?

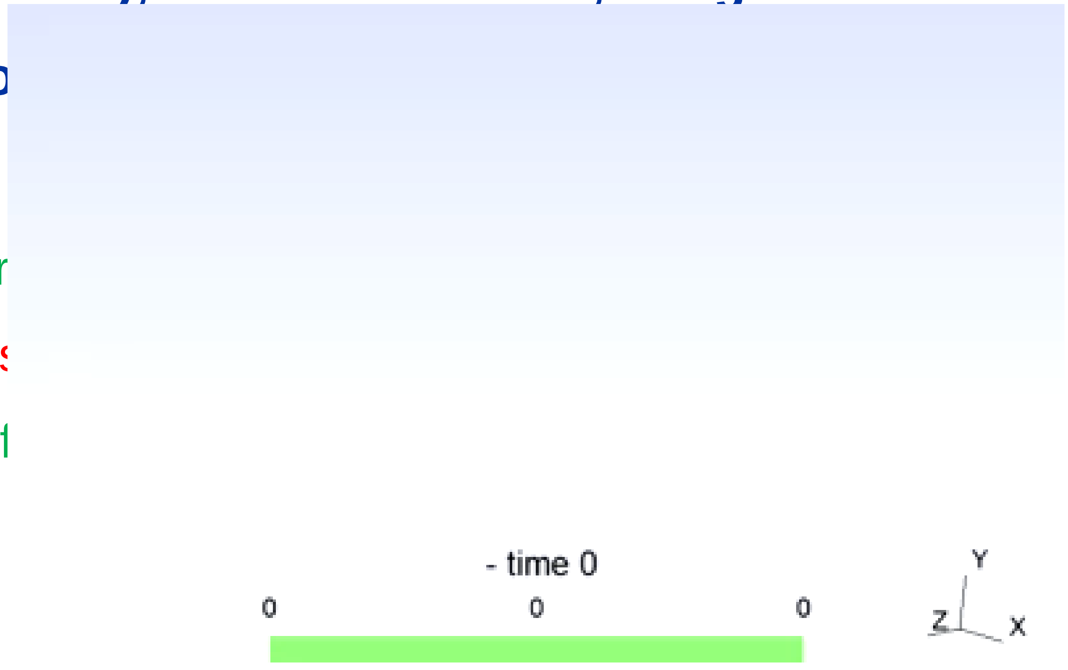
- **Goal: quench behavior simulation of superconducting magnets (LTS and HTS)**
  - Complicated geometries carrying eddy and screening currents
- **Alternatives: partial element equivalent circuits (PEEC), finite differences, integral equatio... ...vart techniques, spectral metho...**
- **This w... ...E-based simulations**



  - **...neral:** FE ... ...le geometrical details, non-linear...
  - **Expensive:** FE’s high approximative capabilities makes...
  - ...rce and free finite element f...
  - ...equire deep understanding...



➤ **Purpose-built FE quench simulation tool based...**



Eddy currents in the inner former

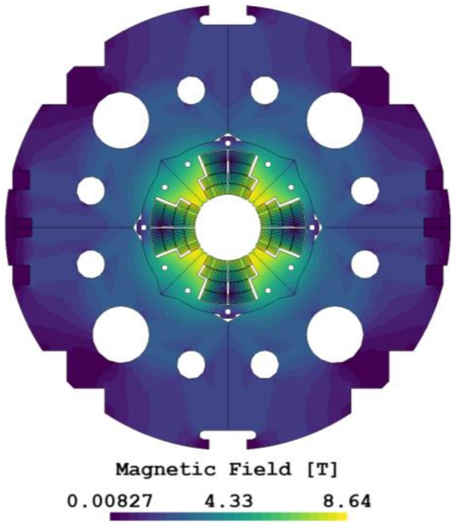
M. Wozniak et al., "Quench Co-Simulation of Canted Cos-Theta Magnets," IEEE TAS (2023)

Finite Element Quench Simulator

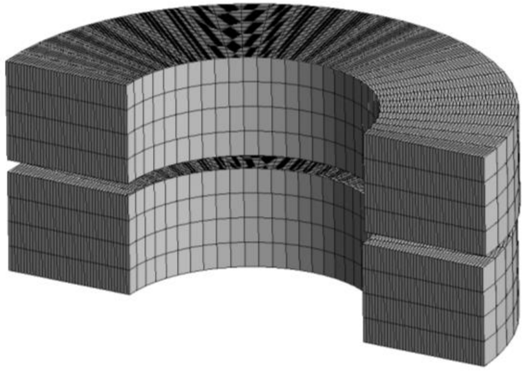
- **FiQuS is an open-source and free to use Python tool.**
- **It's based on open-source FE framework Gmsh/GetDP.**
  - Adding some functionality creates **CERNGetDP as FiQuS's dependency**.
- **It's part of the STEAM framework.**

onelab.info

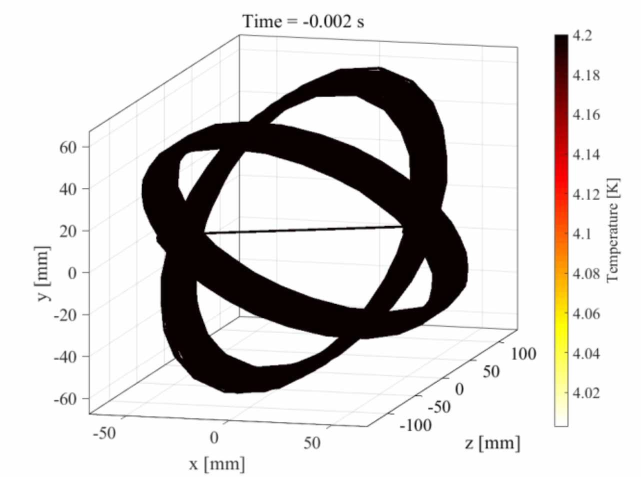
Multipole magnets (MQXA)



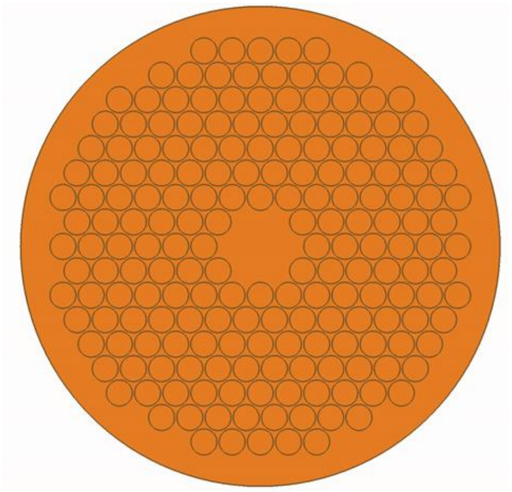
No-Insulation HTS pancake coils



CCT magnet
co-simulation with LEDET

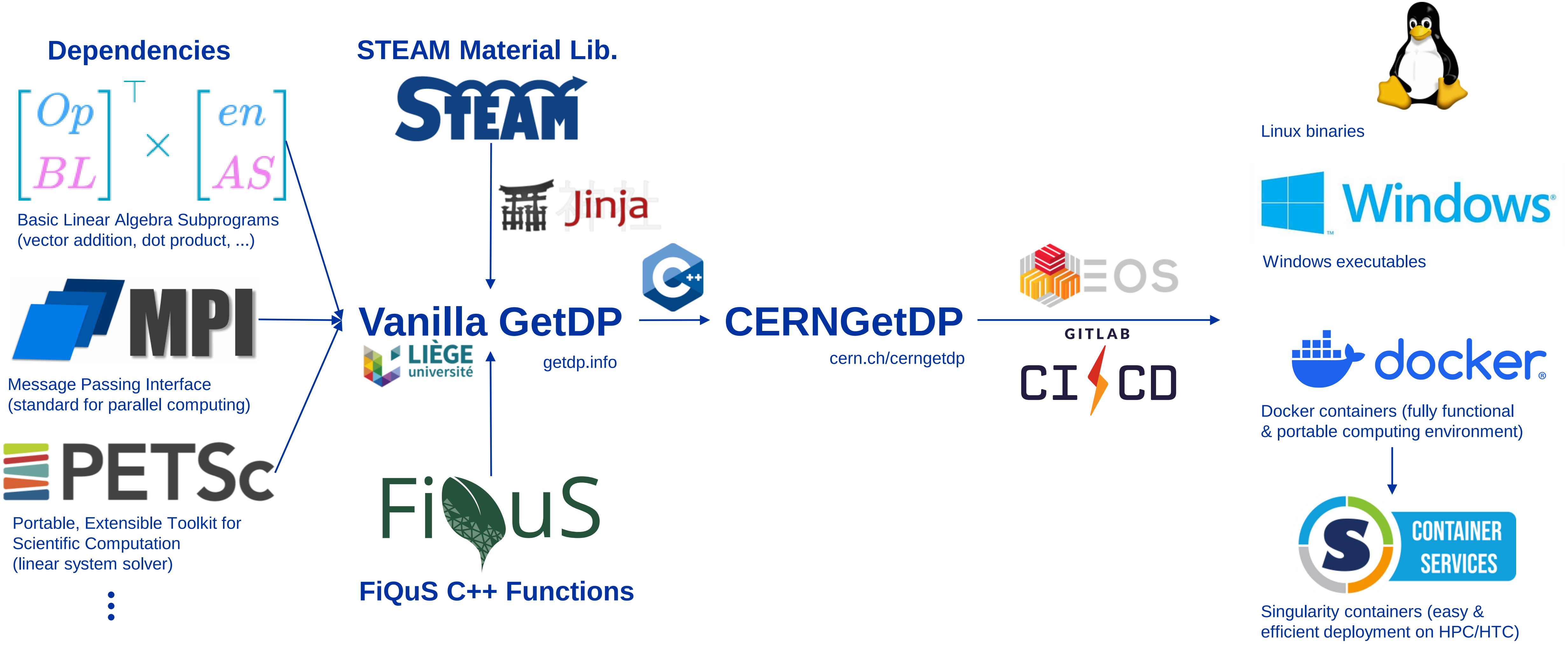


Conductors (wires, cables)



Courtesy of S. Atalay, J. Dular, F. Magnus, E. Ravaioli, A. Vitrano, M. Wozniak

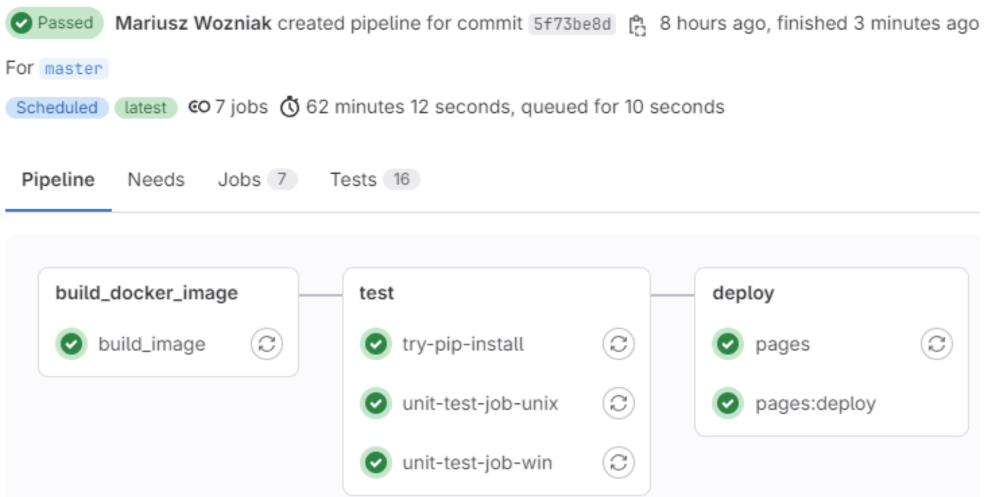
CERNGetDP: Software Toolchain



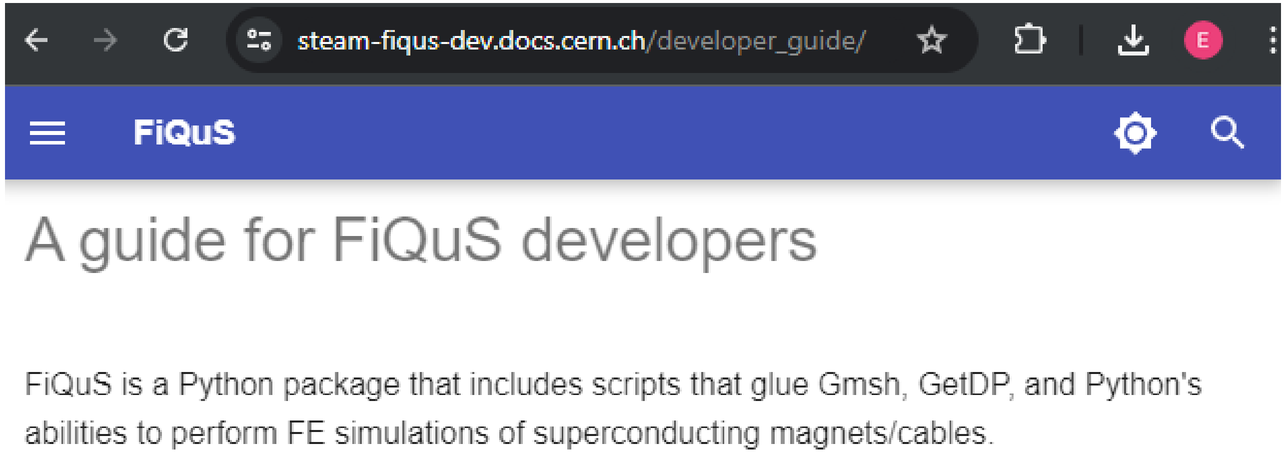
- **Usage of sophisticated open-source (FE) tools requires non-trivial computing environment.**
  - All fully automated on CERN IT-provided runners and FiQuS-managed VMs via CERN Openstack.
  - This way, we can run FiQuS easily on any computing infrastructure we have to (including HPC/HTC).

pipeline passed
coverage 79.00%

FiQuS: Automated Testing, Documentation and Deployment



Gitlab pipeline automatizes mundane jobs such as building software, testing it and deploying the software (e.g., on EOS, pypi, ...) and documentation (e.g., on webpages).



Pipeline automatically creates releases and documentation (from docstrings and Markdown) deployed on webpage.

MkDocs
Project documentation with Markdown.

unit-test-job-unix

13 tests | 0 failures | 0 errors | 100% success rate | 16m 7s

Tests

Suite	Name	Filename	Status	Duration	Details
tests.test_solvers. TestSolvers	test_Pancake3D		✓	6m 4s	View details
tests.test_FiQuS. TestFiQuS	test_01_GenerateAllGeometryOnly		✓	3m 52s	View details

Pipeline (py)tests ensure the consistency of the remote repository.

pytest

... and produce coverage report (what percentage of code am I testing?)

Coverage for **fiqus/data/DataConductor.py**: 100%

157 statements | 157 run | 0 missing | 0 excluded

« prev ^ index » next coverage.py v6.4.4, created at 2024-06-24 16:24 +0200

```
from pydantic import BaseModel, Field
from typing import Union, Literal, Optional

# ------------------ Jc fits --------------------------#
class ConstantJc(BaseModel):
    """
    Level 3: Class for setting constant Jc
    """

    type: Literal["Constant Jc"]
    Jc_constant: Optional[float] = None  # [A/m^2]
```

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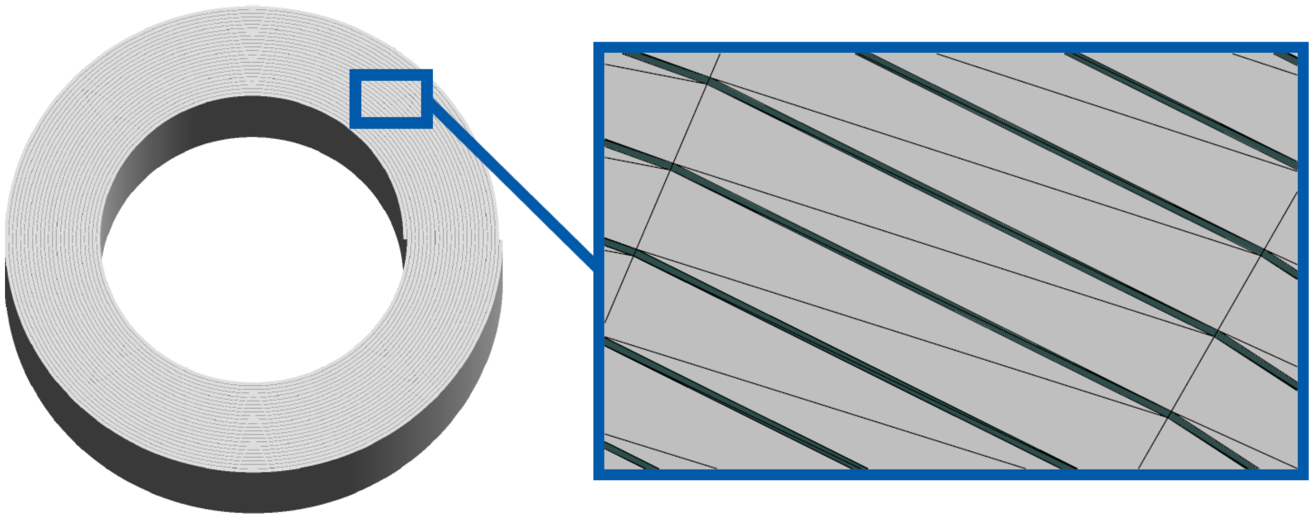
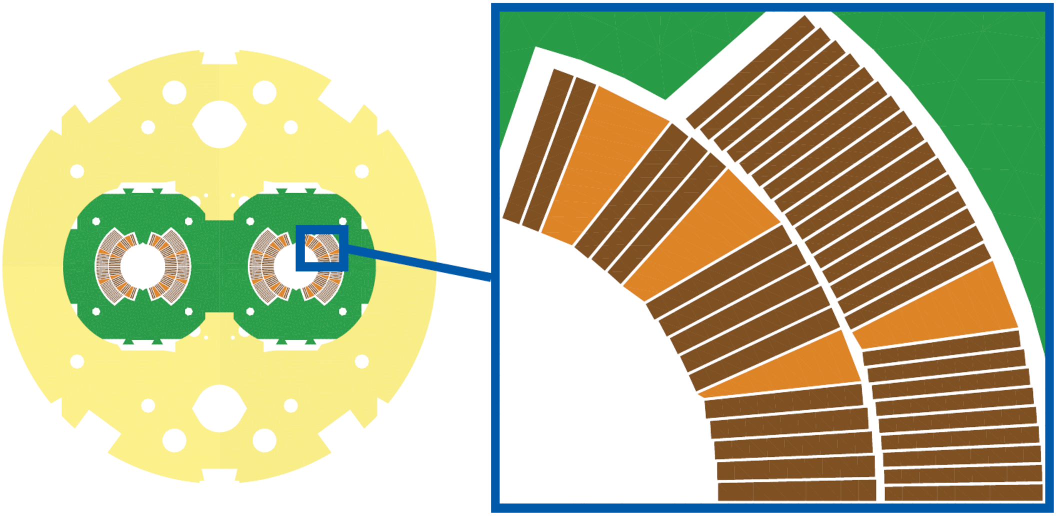
Thin Shell Approximation: Motivation I



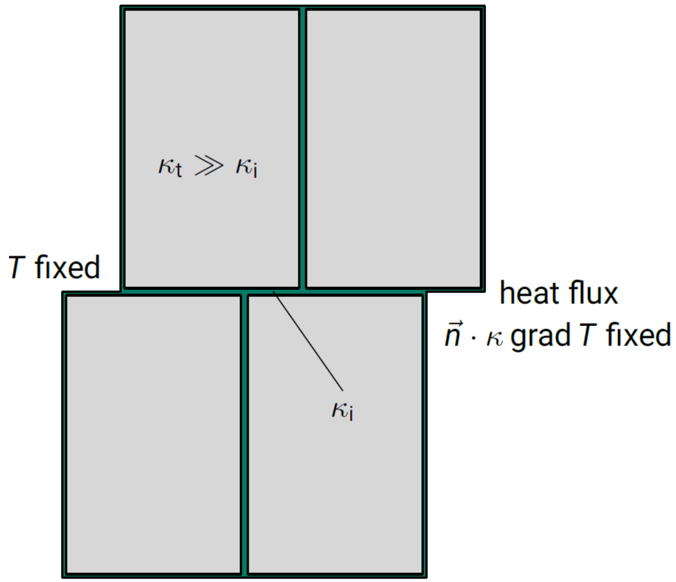
Contact layers in HTS pancake coils

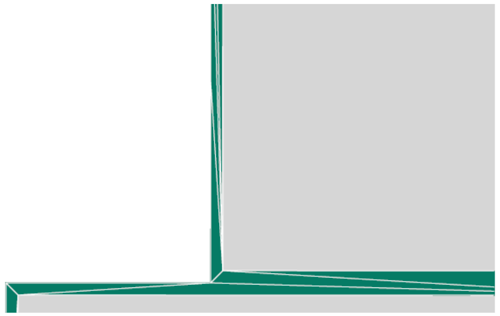


Insulation layers in LHC magnets

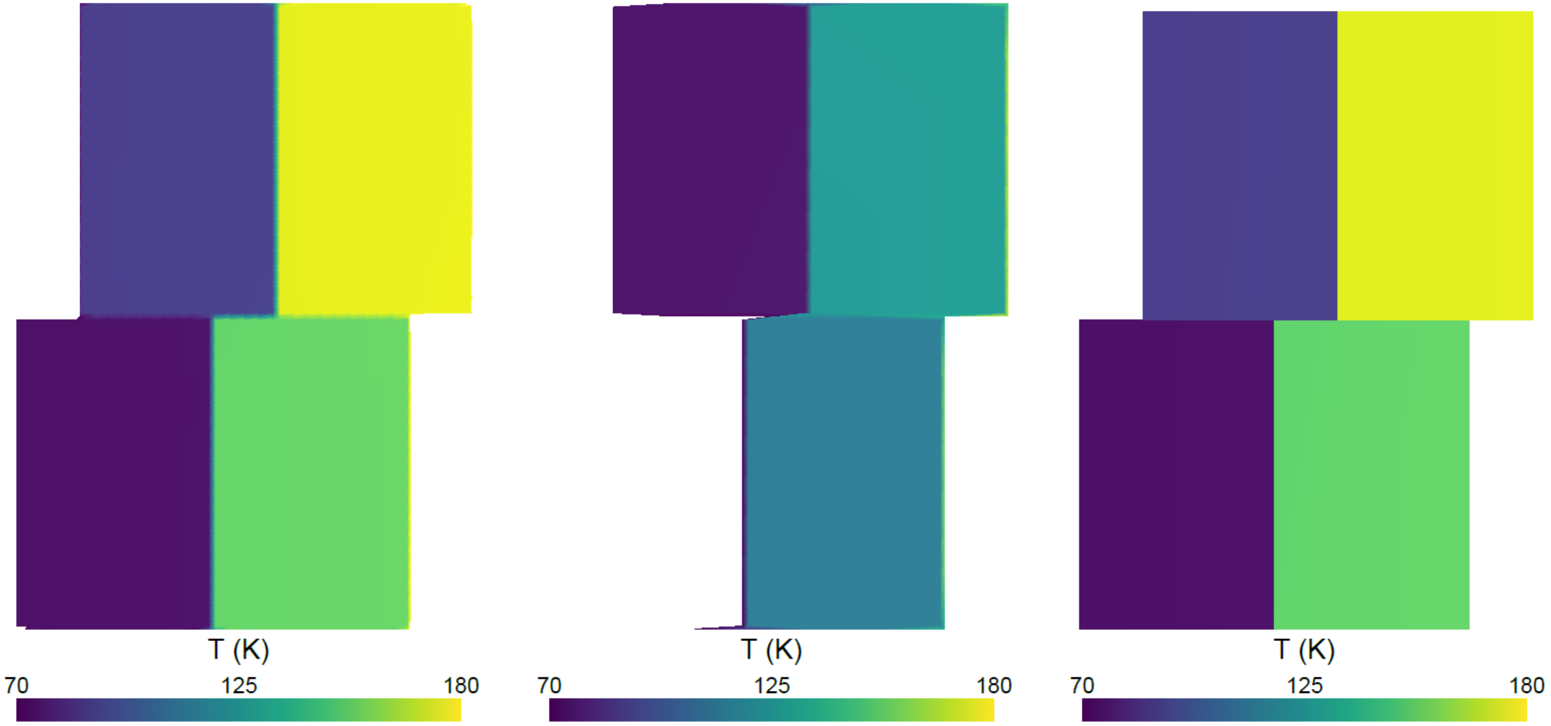
- **Thin layers appear frequently in superconducting magnets.**
  - Their accurate modelling is essential to capture the right transient behaviour.
- **Classical FE modelling leads to many unknowns or low mesh quality.**
  - ➢ Thin shell approximations (TSA) avoid these problems.

Thin Shell Approximation: Motivation II





- **Linear, stationary heat diffusion equation → simple!**
  - Yet, completely wrong results with naively chosen mesh.

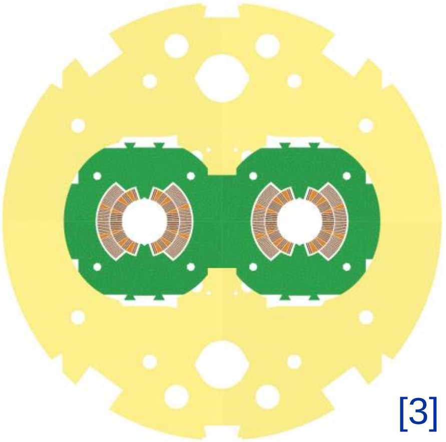


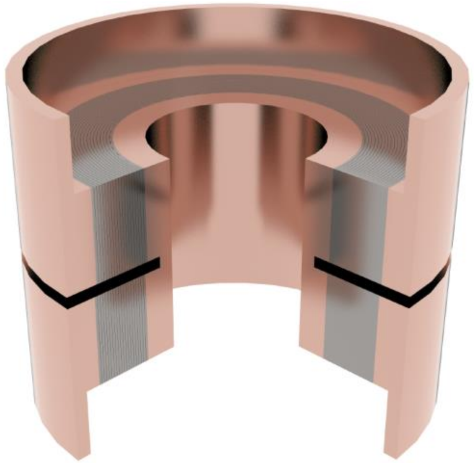
Structured mesh (1400 DoF) Unstructured mesh (38 DoF) Thin shell (30 DoF)

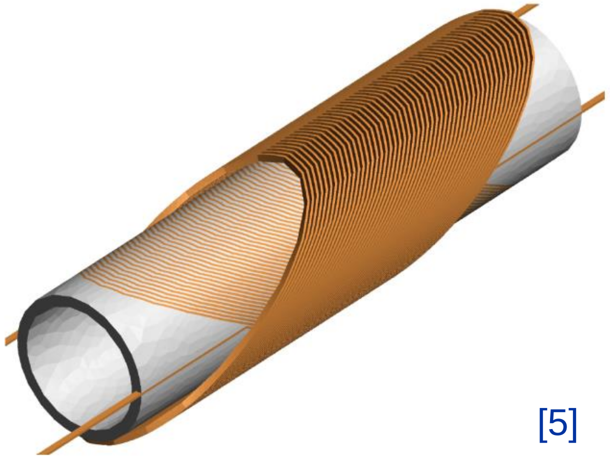
E. Schnaubelt, M. Wozniak, and S. Schöps, "Thermal Thin Shell Approximation Towards Finite Element Quench Simulation", SUST (2023).

TSA Generalities

- **TSA replace volumes with surfaces and appropriate interface conditions.**
  - Many TSA exist in literature, however they are usually only valid for very specific problems. [1]
- **For FiQuS, we needed a general magneto-thermally coupled TSA [2].**
  - General: resistivities from insulating to superconducting, boundary conditions, quench heaters, ...
  - Its generality is best represented by the variety of different models that use the TSA:

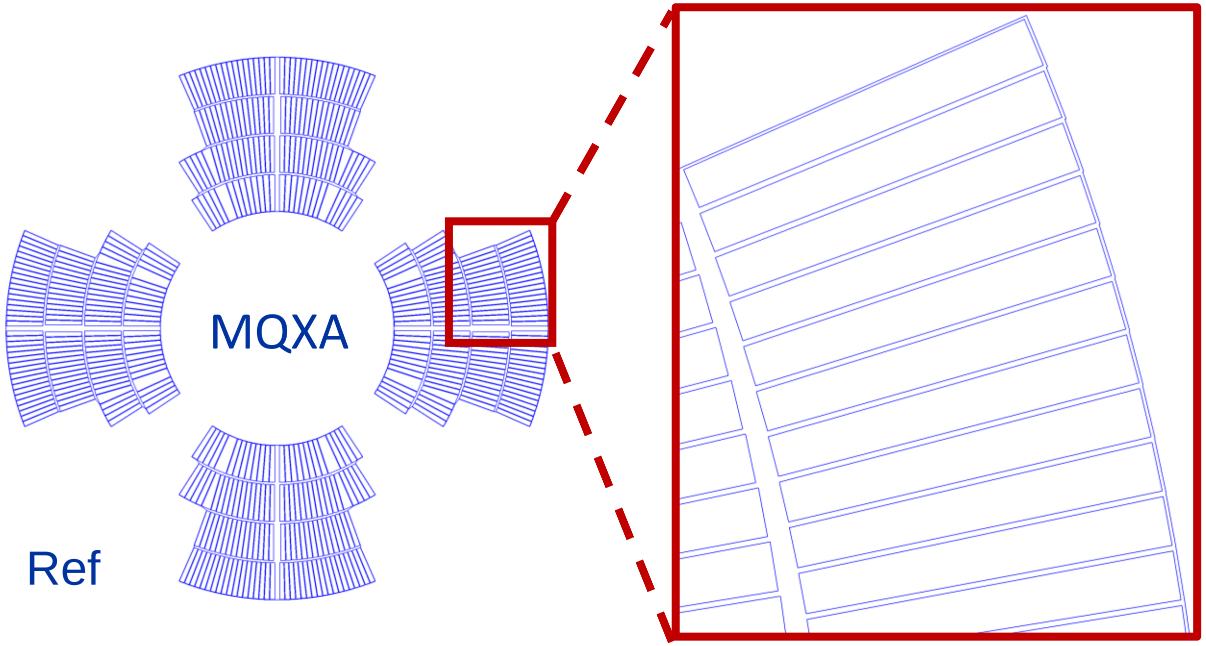

[3]

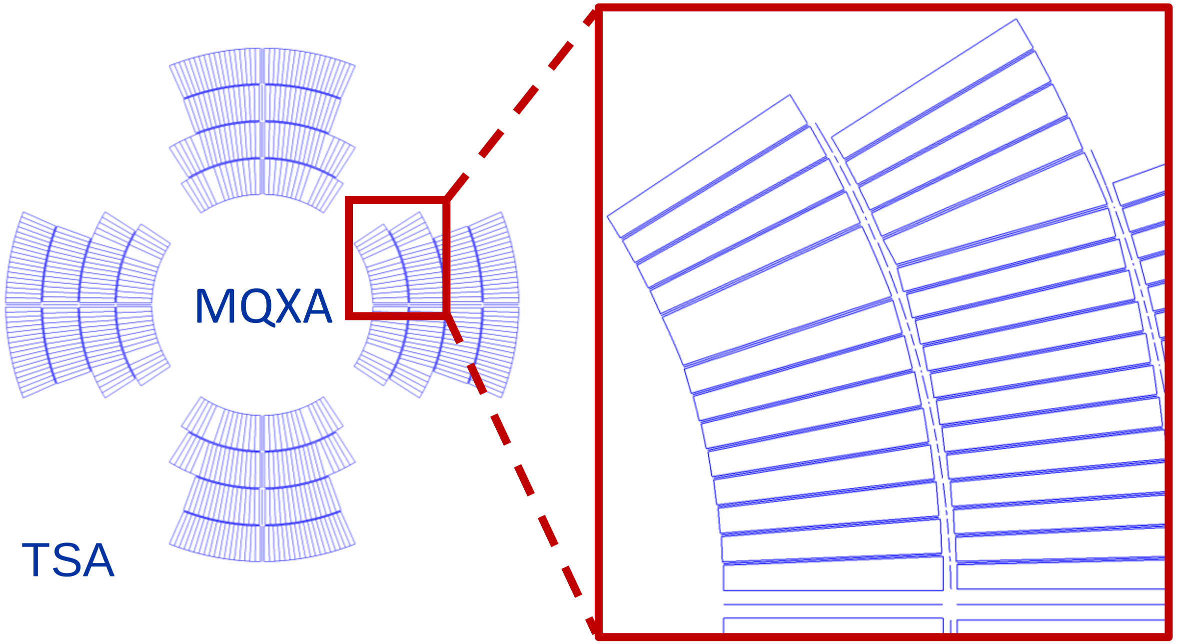

[4]


[5]

[1] B. De Sousa Alves, “3-D Time-Domain Finite Element Modeling of Nonlinear Conductive and Ferromagnetic Thin Films,” Ph.D. thesis, Polytechnique Montréal (2021)
[2]: E. Schnaubelt et al., "Magneto-Thermal Thin Shell Approximation for 3D Finite Element Analysis of No-Insulation Coils," IEEE TAS (2024)
[3]: A. Vitrano et al., "An Open-Source Finite Element Quench Simulation Tool for Superconducting Magnets," IEEE TAS (2023)
[4]: S. Atalay et al., "An open-source 3D FE quench simulation tool for no-insulation HTS pancake coils," SUST (2024)
[5]: M. Wozniak et al., "Quench Co-Simulation of Canted Cos-Theta Magnets," IEEE TAS (2023)

FiQuS-Multipole: Thermal Transient TSA



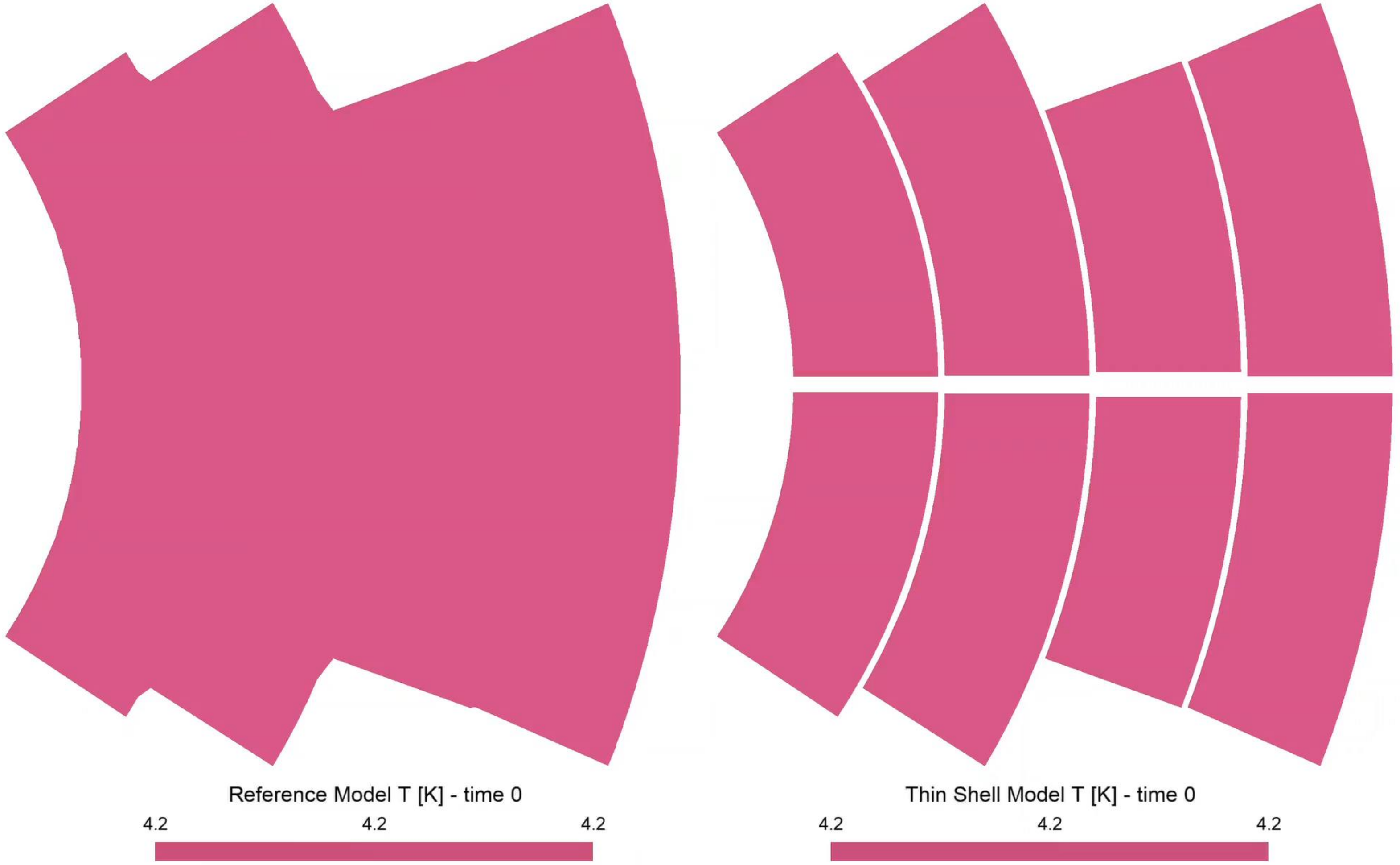


- **Insulation layers are modelled via TSA, represented by mesh lines above.**
  - Handles quench heaters (possible between any half-turns/wedges, also across layers).
  - Handles Helium convective cooling boundary condition via heat transfer coefficient from SMaLi.
- **FiQuS ideology: constructed automatically from .yaml and Roxie input files.**
  - No manual intervention needed (easily reproducible!) → **Dedicated talk by Andrea in July!**

FiQuS-Multipole: TSA Verification

- Constant current, thermal transient, adiabatic conditions, quench imposed in one half turn.

Reference:
77’380
DoFs



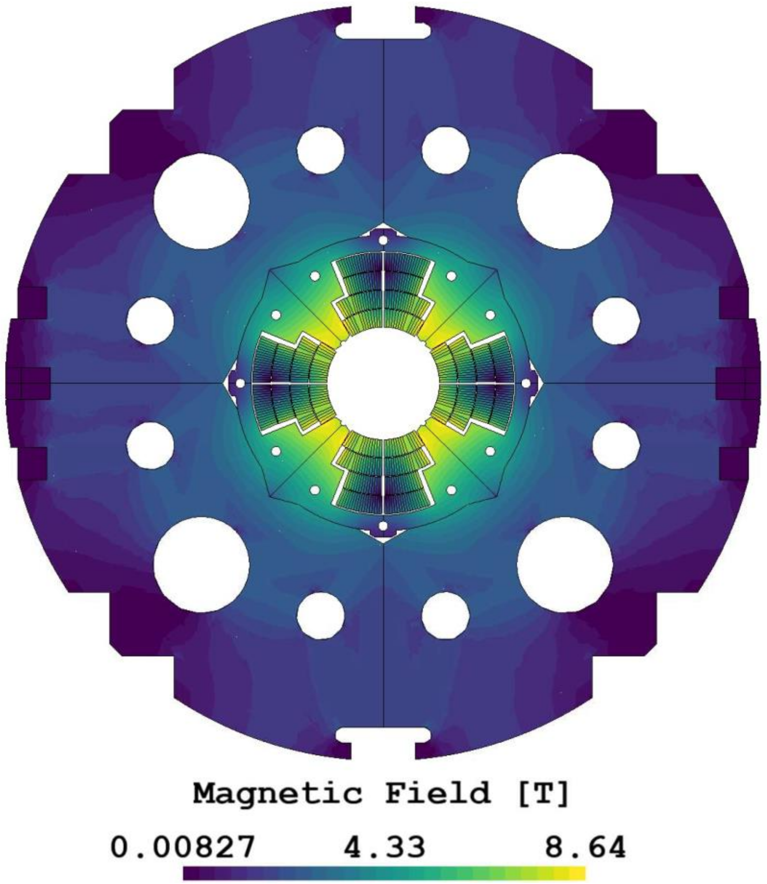
TSA:
13’143
DoFs

~10 times shorter solution time!

A. Vitrano et al., “Finite Element Thermal Thin Shell Approximation for Simulation of Transients in Accelerator Magnets”, CHATS 23.

FiQuS-Multipole: Some Remarks

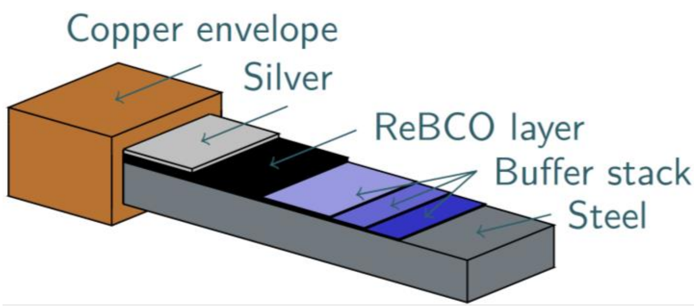
- **Thermal transients are already coupled to magnetostatic solution from FiQuS-Multipole.**
  - Ready for extension to magnetodynamic case including AC loss model via homogenization.
- **Proper verification study reference versus TSA ongoing and to be published.**
  - Verification for quench heater (QH) model for simple model (for real magnet, QH modelled with classical FE without TSA infeasible!)
- **Different magnet types (block-coils, asymmetric coils, HTS-LTS, common-coils, mono cable magnets, ...)**
  - See Andrea's talk in July!
- **Many thanks to Andrea & Mariusz for the collaboration!**

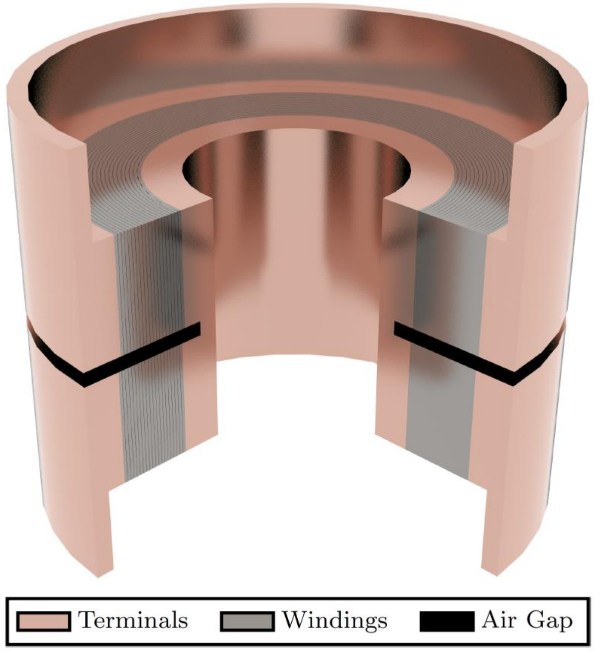


A. Vitrano et al., "An Open-Source Finite Element Quench Simulation Tool for Superconducting Magnets," IEEE TAS (2023)

FiQuS-Pancake3D: Introduction

- **HTS Coated Conductors (CC) wound in spiral turns with or without turn-to-turn (T2T) insulation.**
- **Case without T2T insulation called no-insulation (NI) coils.**
  - Radial T2T currents can circumvent local defects → increased stability.
  - Vanishingly thin electric and thermal T2T contact layers (T2TCL) determine dynamic behavior.
- **Detailed 3D models resolving each turn on the mesh level are needed to analyze complex magneto-thermal transients.**
  - FiQuS-Pancake3D creates these fully automated and parameterized.
  - All detailed features: remember Sina's section talk?

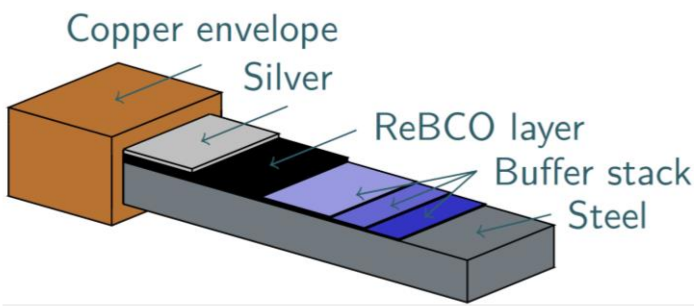




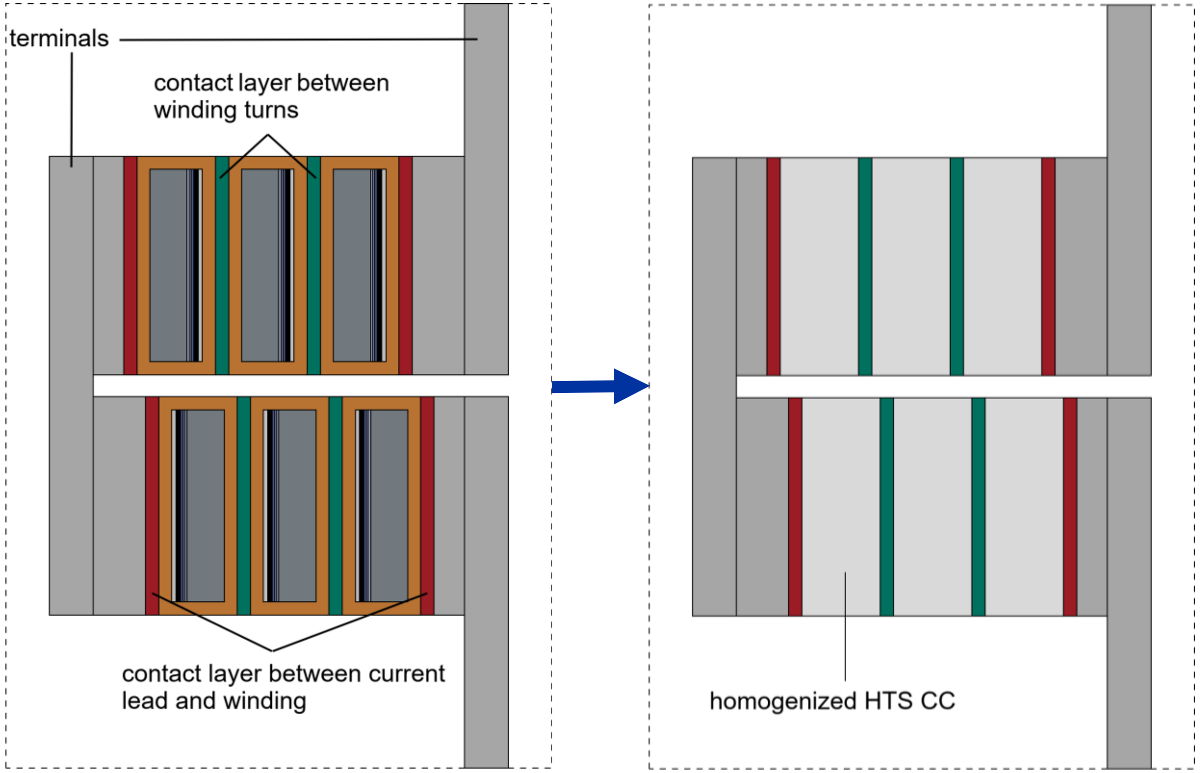
S. Atalay et al., "An open-source 3D FE quench simulation tool for no-insulation HTS pancake coils," SUST (2024)

FiQuS-Pancake3D: Homogenized HTS CC

- **Magneto-thermal coupled model.**
- **Each turn is resolved on the mesh level.**
- **The HTS CC is homogenized.**
  - Power law with angle dependency for HTS.
  - Anisotropic homogenization different in radial (layers in series) and axial/azimuthal direction (layers in parallel).
  - In particular, current sharing is resolved.
- **Screening currents naturally considered thanks to FE magnetodynamic model.**



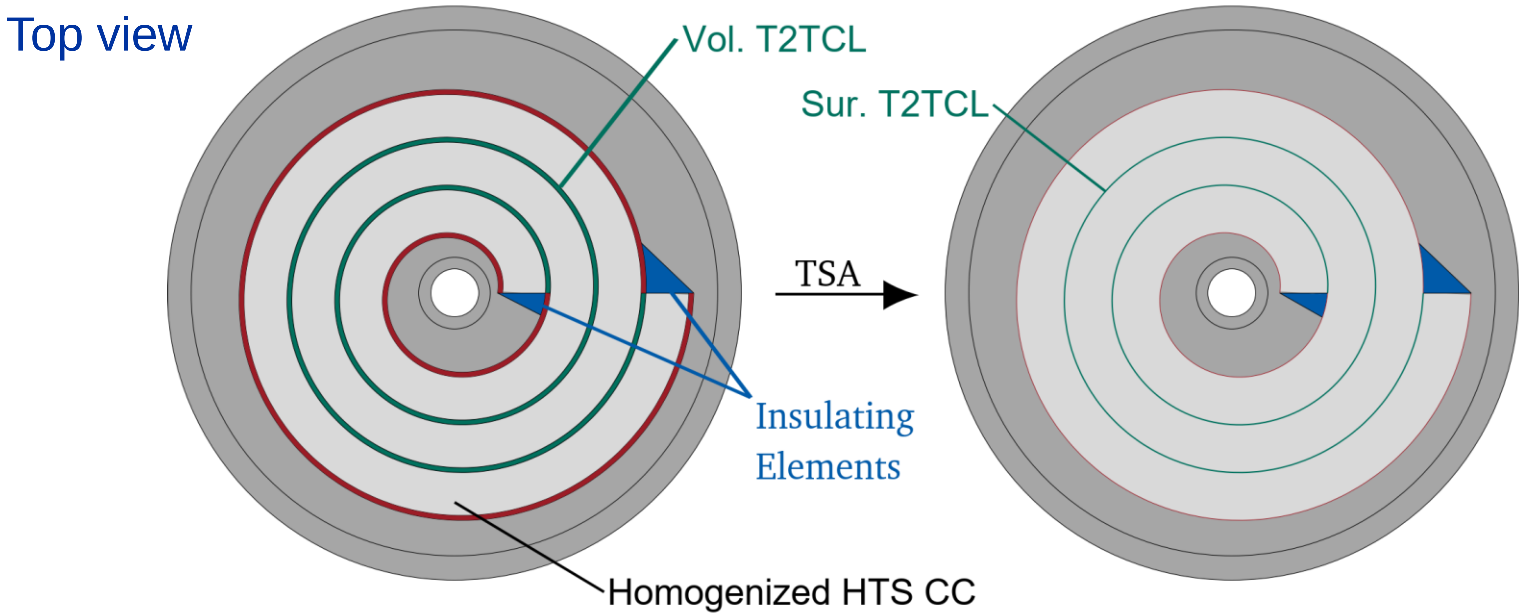
Side view



E. Schnaubelt et al., "Magneto-Thermal Thin Shell Approximation for 3D Finite Element Analysis of No-Insulation Coils," IEEE TAS (2024)

FiQuS-Pancake3D: Magneto-Thermal TSA

- **Volumetric T2TCL is replaced by a surface modelling equivalent physical phenomena.**
  - It is implemented in an $\vec{H} - \phi$ formulation coupled to the heat diffusion equation.
  - The special case of insulated pancakes is covered as well.

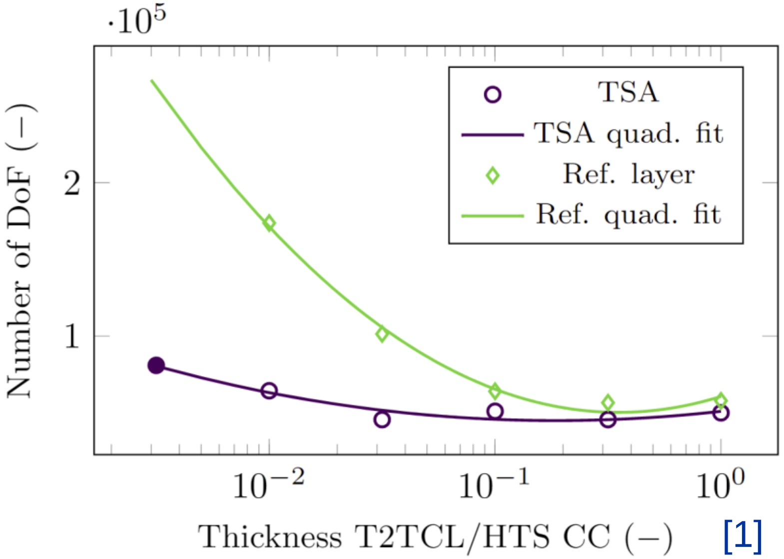


E. Schnaubelt et al., "Magneto-Thermal Thin Shell Approximation for 3D Finite Element Analysis of No-Insulation Coils," IEEE TAS (2024)

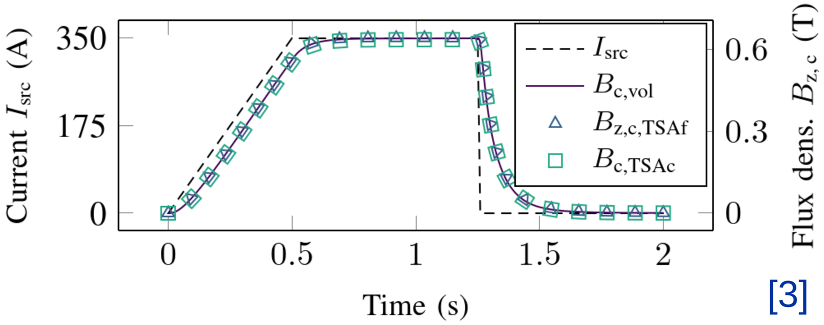
FiQuS-Pancake3D: Systematic Verification

- **Systematic verification against classical FE with volumetric T2TCL [1,2,3] shows excellent agreement.**
  - Also for radial and azimuthal currents [2]

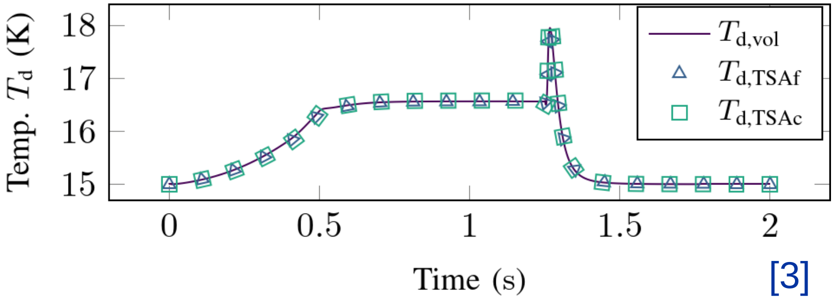
- **TSA outperforms the reference, especially the thinner the T2TCL the higher the gain.**
  - Also simpler to mesh!



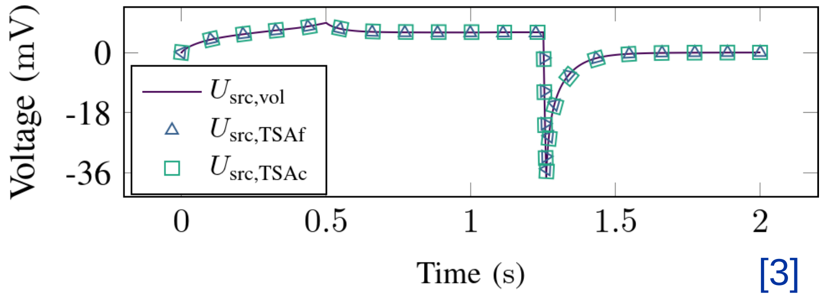
[1]



[3]



[3]

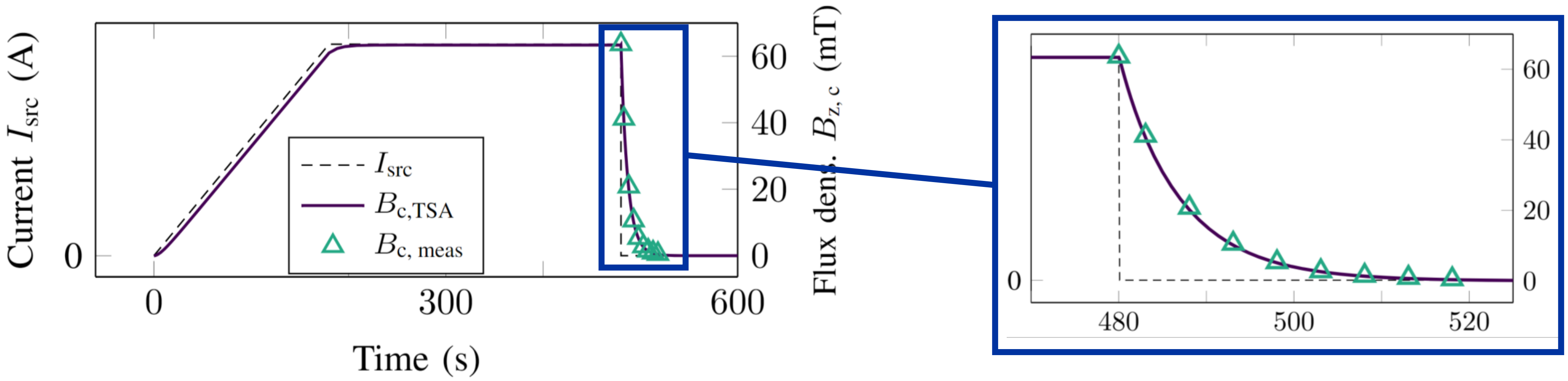


[3]

[1]: E. Schnaubelt et al., "Thermal [TSA] Towards [FE] Quench Simulation", SUST (2023)
[2]: E. Schnaubelt et al., "Electromagnetic Simulation of [NI] Coils Using $\vec{H} - \phi$ [TSA]," IEEE TAS (2023)
[3]: E. Schnaubelt et al., "Magneto-Thermal [TSA] for 3D [FE] Analysis of [NI] Coils," IEEE TAS (2024)

FiQuS-Pancake3D: Partial Validation

- **Comparison against sudden discharge measurements from [1]**
- **50 turns NI coil, 80 mm inner diameter**
  - Measured characteristic time 7.14 s → contact resistance 11.2 μΩcm^2



[1]: J. Lee et al., “Investigation on the Electrical Contact Resistance of Soldered Metal Insulation REBCO Coil,” IEEE TAS (2021).

E. Schnaubelt et al., “3D Magneto-Thermal FE Simulations of NI HTS Coils with Thin Shell Approximations”, EUCAS’23 Oral Presentation.

Cooling applied to copper terminal ports.

$\vec{J}$ (A/m^2)

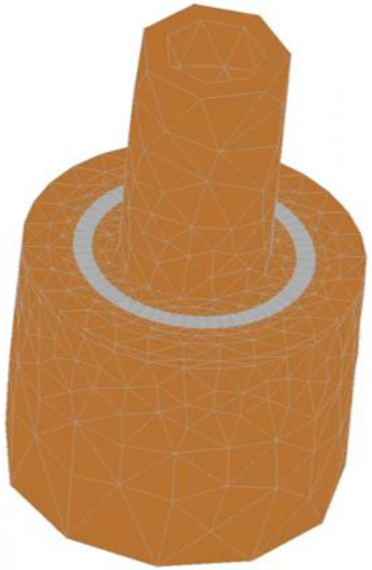
$5 \cdot 10^5$ $5 \cdot 10^6$ $5 \cdot 10^7$ $5 \cdot 10^8$

T (K)

15 16

$\vec{B}$ (T)

0 0.2 0.4

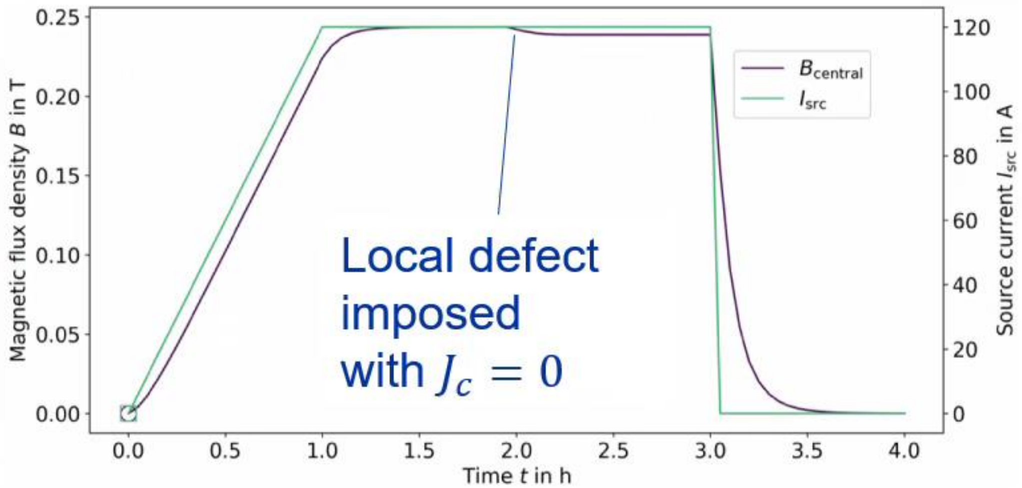


$\vec{J}_{\text{radial}}$ (A/m^2)

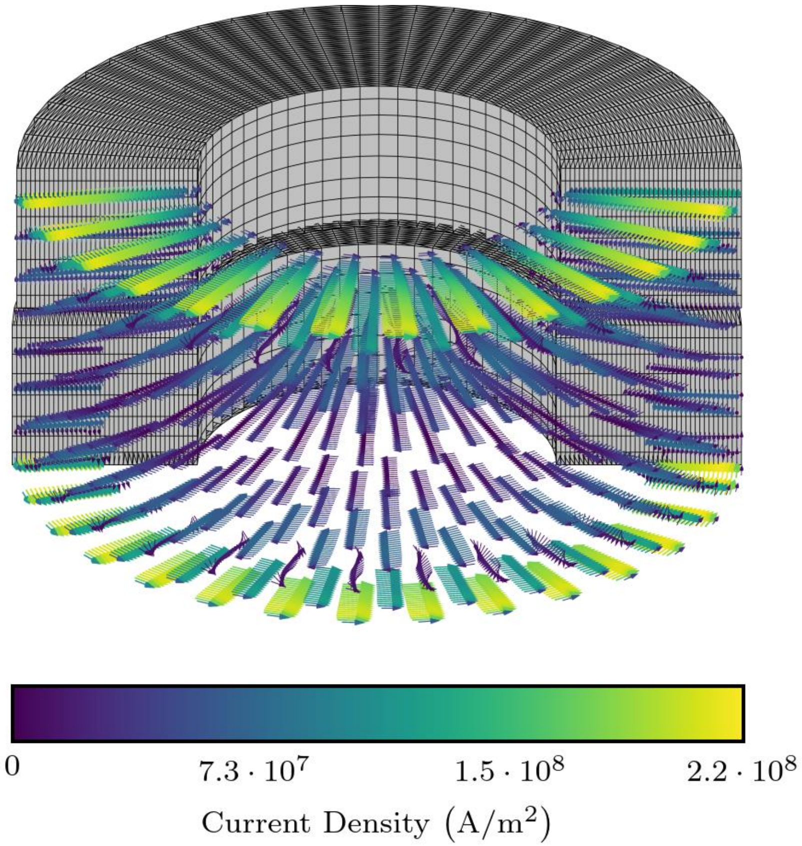
$4 \cdot 10^3$ $4 \cdot 10^5$

$\vec{J}_{\text{angular}}$ (A/m^2)

$5 \cdot 10^7$ $5 \cdot 10^8$

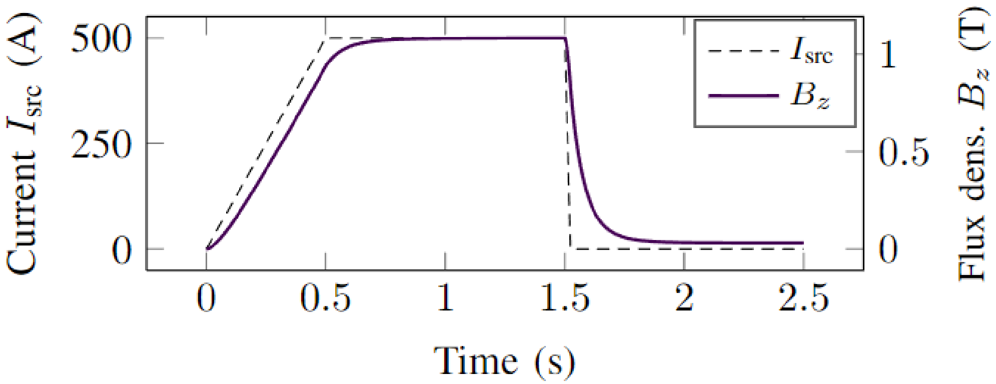


FiQuS-Pancake3D: Stacks and Magnetization

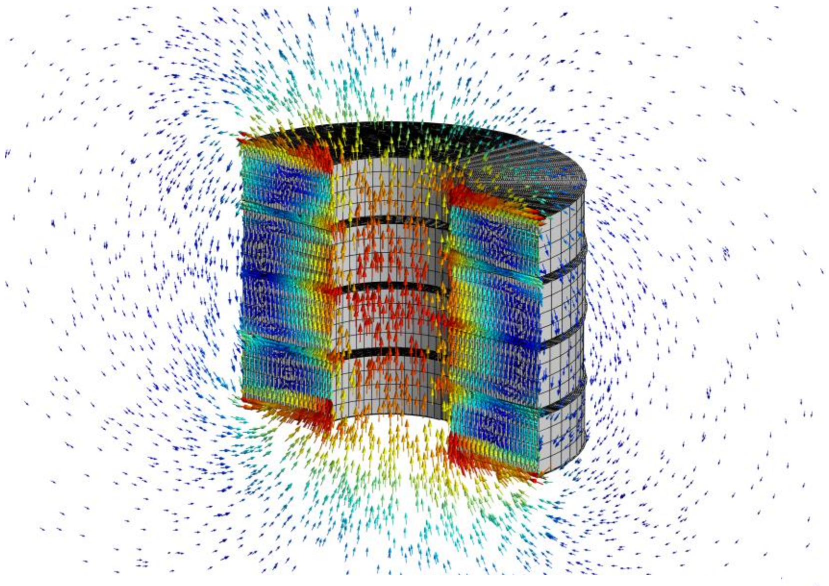


Screening currents in a 2-pancake stack [1]

Non-zero magnetic field after power supply turned off [2]

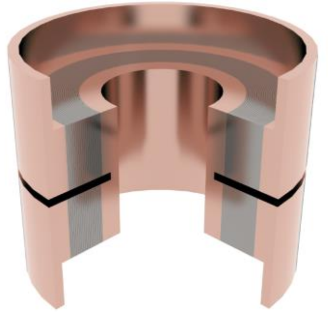


$\vec{B}$-field of 4-pancake stack [1]



[1]: S. Atalay et al., "An open-source 3D FE quench simulation tool for no-insulation HTS pancake coils," SUST (2024)
[2]: E. Schnaubelt et al., “Electromagnetic Simulation of No-Insulation Coils Using $\vec{H} - \phi$ [TSA]," IEEE TAS (2023)

FiQuS-Pancake3D: Some Remarks

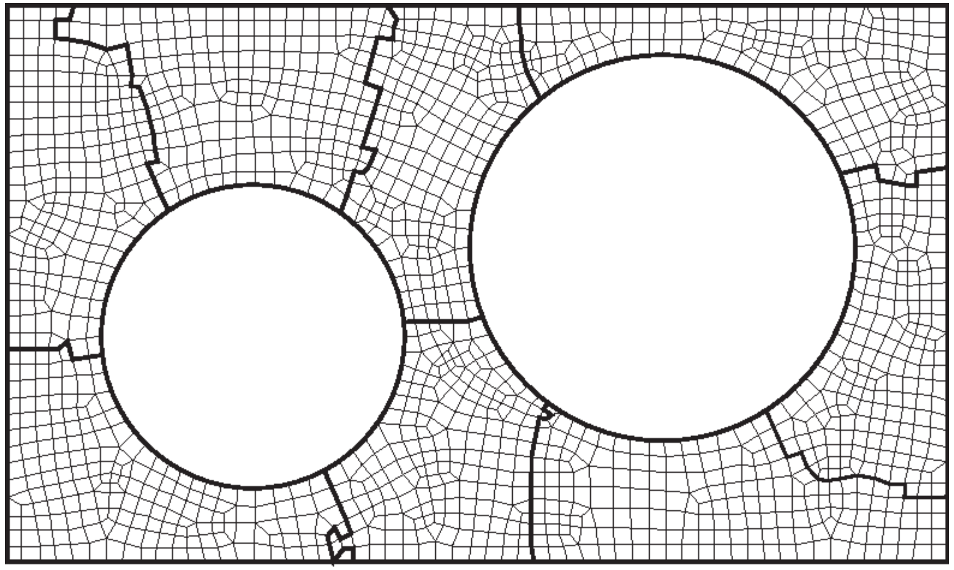


- **Geometries should be extended to more general geometries (racetrack, cloverleaf, ...) from generic CAD or OPERA conductor files.**
- **Methods to reduce computational complexity are needed.**
  - General 3D: parallelization methods on HPC clusters (see next slides).
  - Model specific: reduced order methods (e.g., 2D) or homogenized models
- **Systematic validation against measurements including temperature**
  - This needs properly and comprehensively reported measurements (no fudge factors!).
- **Many thanks to Sina, Julien and Mariusz for the collaboration!**

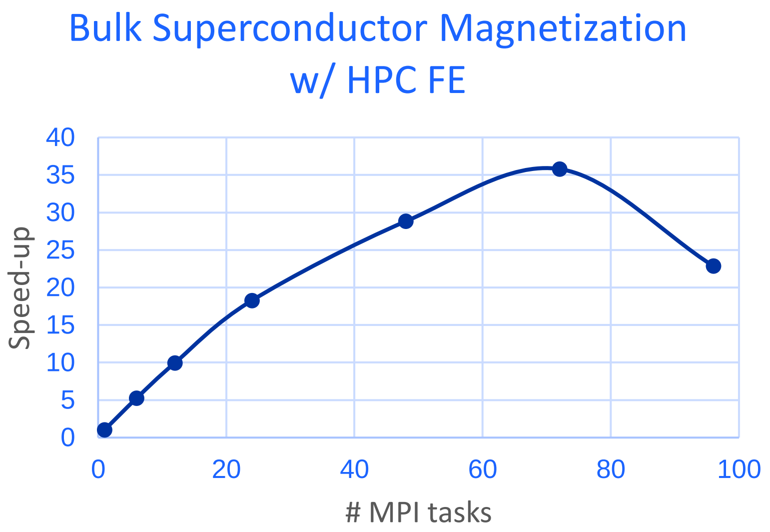
Outline of the Talk

Parallelization: Some General Remarks

- **3D FE leads to big systems → ~ millions of DoF for magnetodynamic problems.**
  - Time integration of highly nonlinear problem needed → practical computational times?
- **Modern FE makes heavy use of parallelization in space and (less intuitive) time.**
- **Split computational domain and solve problem on subdomains concurrently.**
  - The clue of the method is to glue the sub-domain solutions back together for global consistency.



G.P. Nikishkov, "Basics of the Domain Decomposition Method for Finite Element Analysis", in F. Magoulès, (Ed.), "Mesh Partitioning Techniques and Domain Decomposition Methods", Saxe-Coburg Publications, 2007.

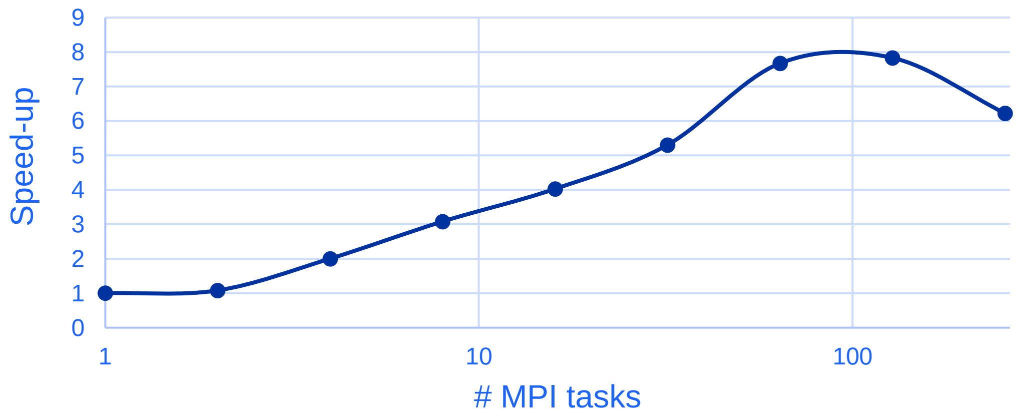


Data from M. Olm et al., "Simulation of High Temperature Superconductors and experimental validation," Comput. Phys. Commun. (2019)

FiQuS-Pancake3D: Some Parallelization Results

- **Parallel-in-time integration splits time domain in subdomains and integrate concurrently**
  - Specific update formula and iterative scheme ensures global consistency.
  - For magneto-thermal current ramp of NI coil: moderate speed-up of 2.75 for 16 subdomains [1]
  - More specific research needed for highly non-linear quench problem, simplified problem discussed in [2]

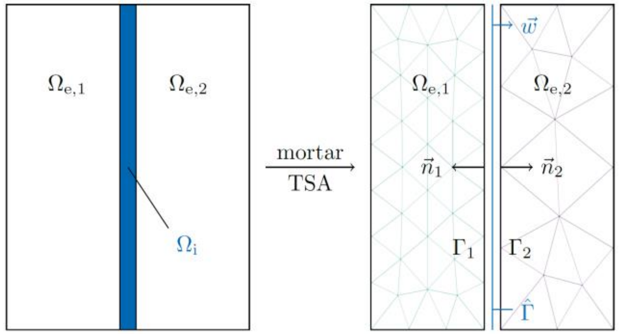
- **GetDP compiled with MPI has some first parallelization capability itself.**
  - Speed-up of around 8 with 64 MPI tasks
  - More work needed for ~ ideal linear scaling, this is not yet proper domain decomposition!



[1]: E. Schnaubelt et al., "Parallel-in-Time Integration of Transient Phenomena in No-Insulation Superconducting Coils Using Parareal," SCEE'24 proceedings, submitted
[2]: T. Baumann et al., "Adaptive time step selection for Spectral Deferred Corrections," Springer Numerical Algorithms (2024), submitted

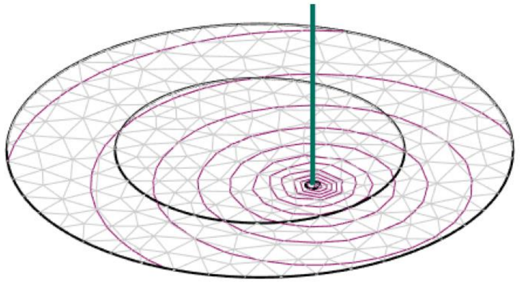
FiQuS: Further Work

- **Mortar TSA removes the need for conforming meshes.**
  - Full meshing freedom → improved efficiency of multipole model
  - Master’s thesis by R. Hahn with paper submitted for publication [1]

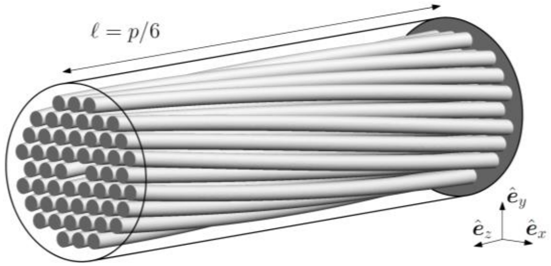


[1]

- **Reduced vector potential removes the need to discretize conductor in mesh [2].**
  - Joint work led by colleagues from TU Darmstadt,
    L. A. M. D’Angelo as lead author


[2]

- **Parallelization efforts benefit all FiQuS models (and even other tools?)**
  - E.g., used to speed up computation of 3D reference for CATI model [3]



[3]

[1] R. Hahn et al., “Mortar Thin Shell Approximation for Analysis of Superconducting Accelerator Magnets,” submitted to SCEE’24 Proceedings.
[2] L. A. M. D’Angelo et al., “Efficient Reduced Magnetic Vector Potential Formulation for the Magnetic Field Simulation of Accelerator Magnets,” IEEE Trans. Magn. (2024).
[3] J. Dular et al., “Coupled Axial and Transverse Currents Method for Finite Element Modelling of Periodic Superconductors”, SUST (2024).

Outline of the Talk

- **Why Finite Elements?**
- **Brief Introduction to FiQuS**
  - CERNGetDP Computing Environment
- **Two FiQuS Models in Detail**
  - Thin Shell Approximations
  - FiQuS-Multipole
  - FiQuS-Pancake3D
- **Early Parallelization in FiQuS**
  - Parallelization in time and space.
- **Conclusion and Outlook**

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Conclusion and Outlook

- **The software toolchains behind FiQuS and CERNGetDP have been introduced.**
- **All discussed tools/models are open-source following CERN’s open science policy.**
- **Two FiQuS models, Multipole and Pancake3D, have been introduced in detail.**
  - **Thin shell approximations** are enabling technologies for both.
  - Particular focus is on **ease-of-use**, **efficiency**, and **reproducibility**.
- **The potential of parallelization and some first results have been shown.**
  - We are just getting started using CERN’s powerful HPC and HTC infrastructure.
- **Outlook: systematic validation against measurements, further HPC improvements, ...**
  - Show and use predictive capabilities for design of experiments.

Thank you for your attention! Special thanks to all collaborators!

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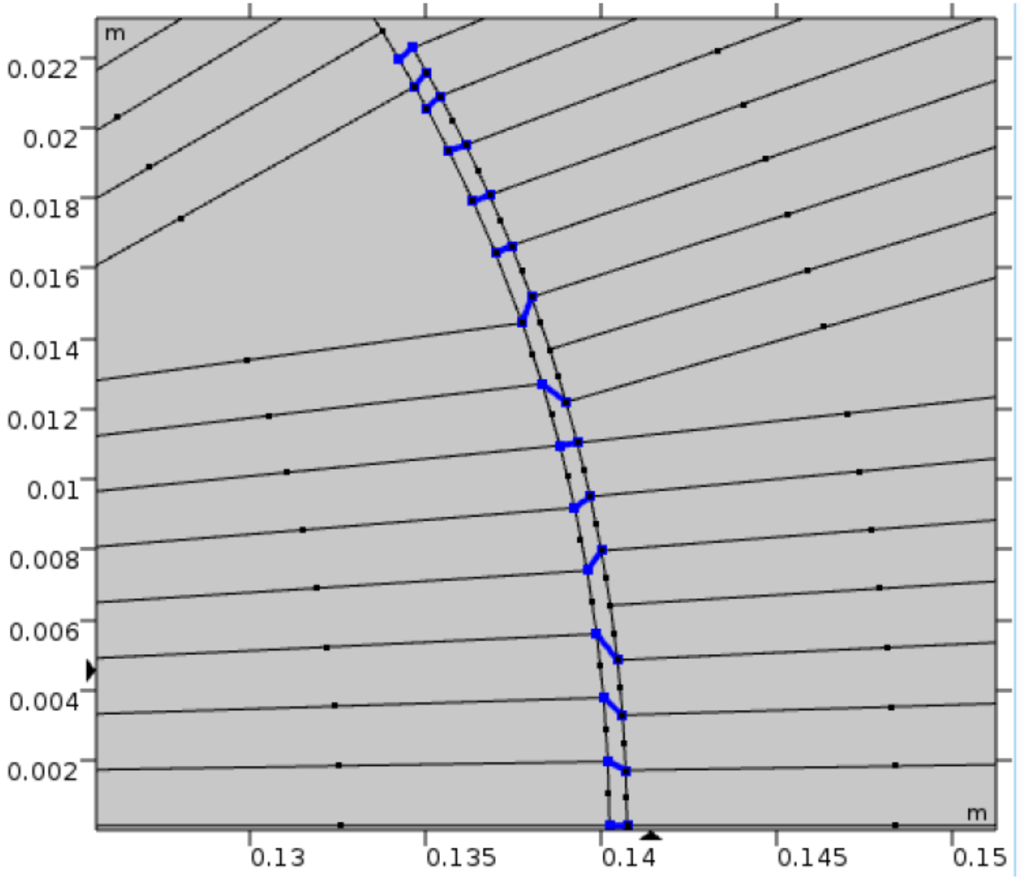
Sigma Non-Automatic Modelling

- **According to Sigma documentation [1] Figure 3.29, mesh lines of infinite resistivity have to be inserted manually.**



[1]: SIGMA documentation v1.2, EDMS 2141579