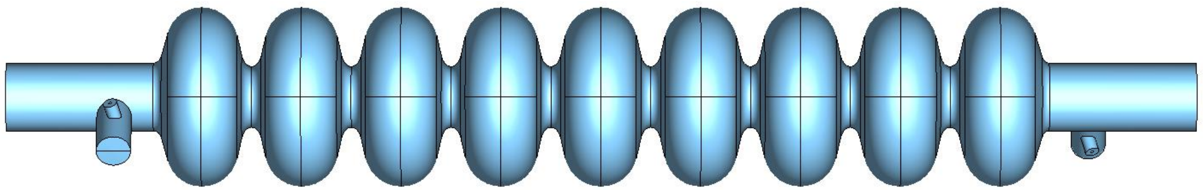
HYBRID TRANSMISSION CONDITIONS FOR THE SCHWARZ DOMAIN DECOMPOSITION METHOD

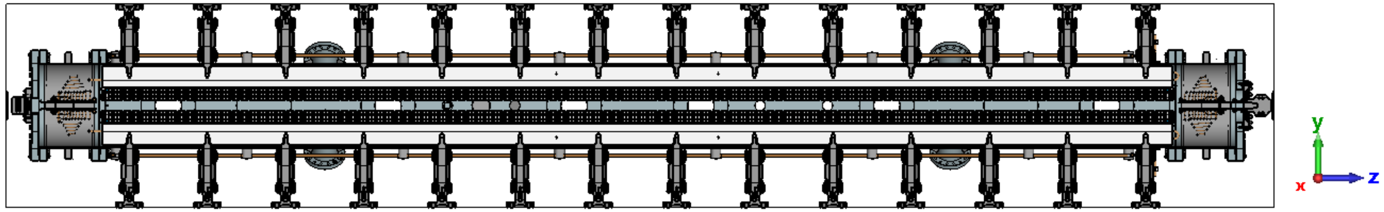
Frederik Quetscher, Erion Gjonaj, Herbert De Gersem

MOTIVATION

Challenges

- Optimization of beam quality and stability is a key task in accelerator design
- Requires accurate simulations for electromagnetically large structures
  - Time consuming
  - Large memory demands



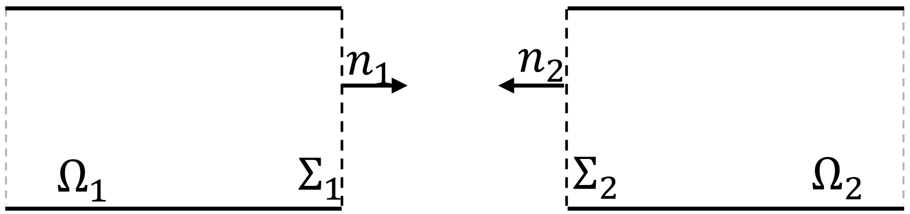


Solution

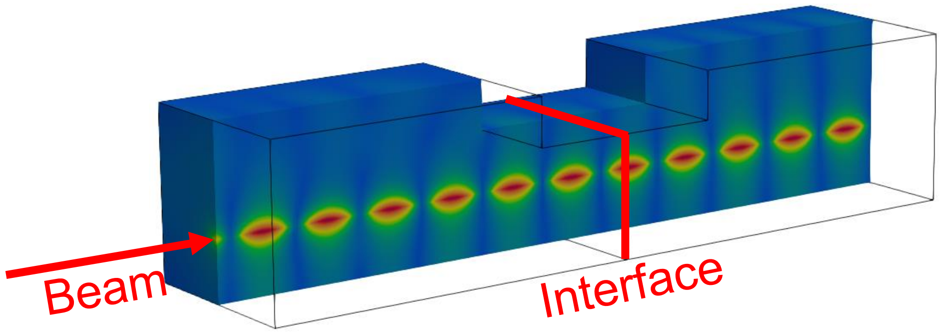
- FEM in frequency domain
  - Promising trade off between computational cost and memory demands
  - Avoids nonlinear eigenvalue problems
- HPC parallelization
- Promising approach:
  Schwarz domain decomposition method

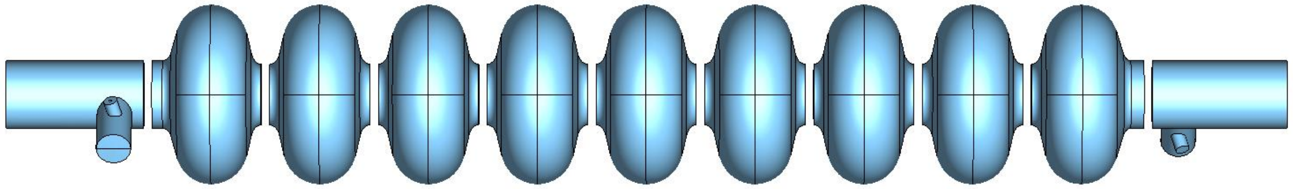
CONTENT

- Schwarz domain decomposition introduction
  - Modal Transmission Condition
- Convergence on Model Problems
  - Hybrid Transmition Condition
- Application to TESLA Cavity
- Update on FFS

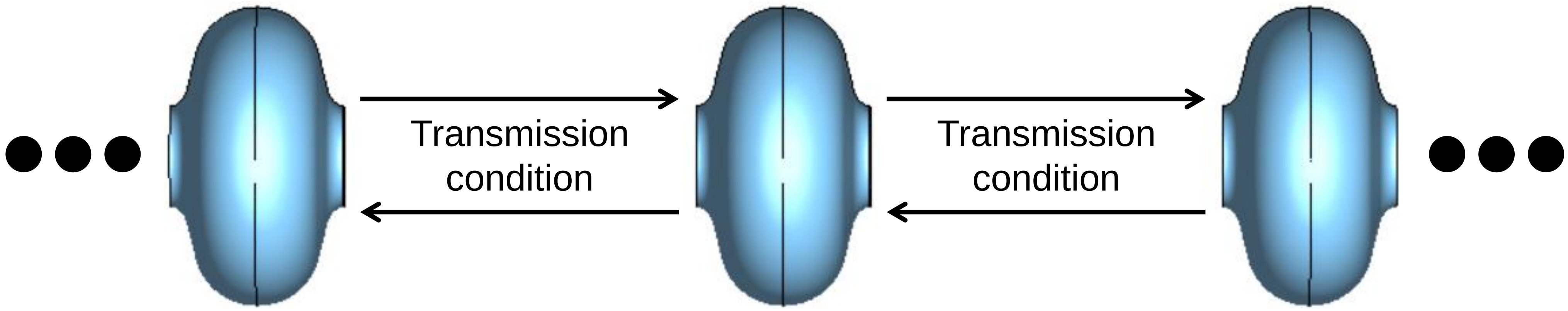


$$\gamma_1^{t}(H_1^2) + \boldsymbol{\Upsilon}\gamma_1^{T}(E_1^2) = -\gamma_2^{t}(H_2^1) + \boldsymbol{\Upsilon}\gamma_2^{T}(E_2^1)$$





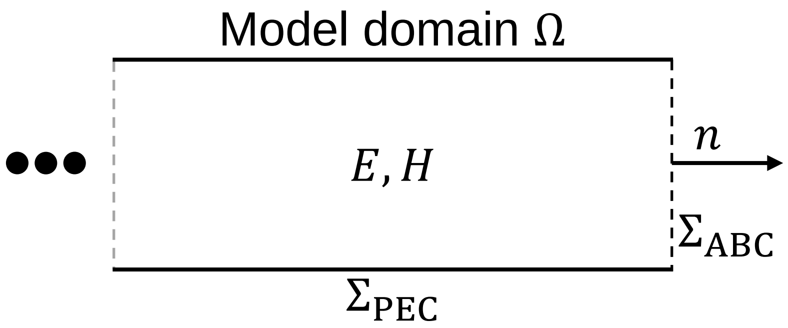
SCHWARZ DOMAIN DECOMPOSITION
OVERVIEW



- Cut model into pieces/domains
- Apply a **transmission condition** at the interfaces
  - Involves an absorbing condition (ABC) at the interface
  - Additionally, exchange outgoing waves as domain excitations
- Iterate until convergence
- Acts as a preconditioner for an iterative solution on HPC platforms

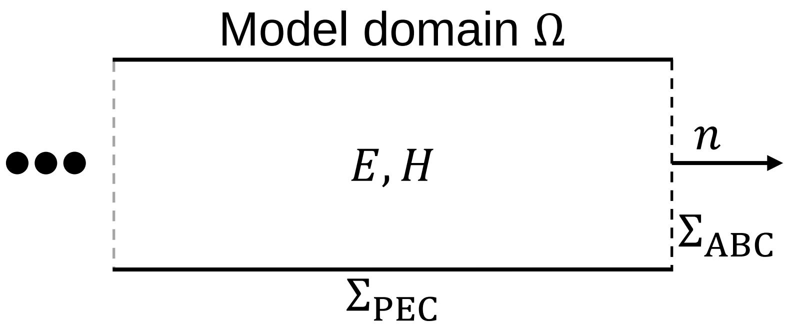
ABSORBING BOUNDARY CONDITIONS
EXACT

- Impedance type boundary condition (IBC)
  - $\gamma^{\mathrm{t}}(H) + \boldsymbol{\Upsilon}\gamma^{\mathrm{T}}(E) = 0$
  - With trace operators
    - $\gamma^{\mathrm{t}}(H) = n \times H,\ \ \gamma^{\mathrm{T}}(E) = n \times (n \times E)$
- Exact admittance operator for planar surfaces
  - $\boldsymbol{\Upsilon} = Y_0(\mathbf{I} + k_0^{-2}\Delta_\perp)^{-0.5}(\mathbf{I} - k_0^{-2}\nabla_\perp \times \nabla_\perp \times)$
- Not directly suitable for a numerical scheme



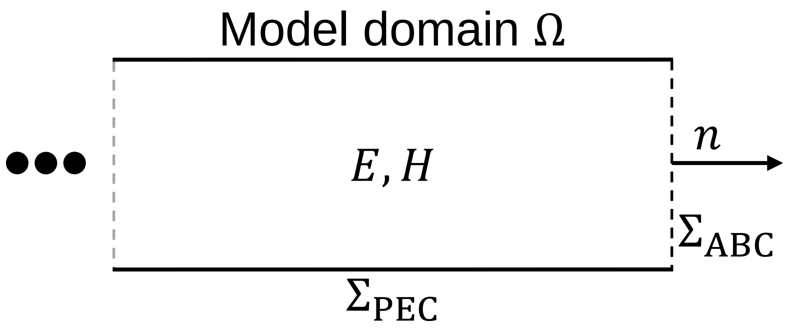
ABSORBING BOUNDARY CONDITIONS
APPROXIMATE

- Exact IBC operator
  - $\boldsymbol{\Upsilon} = Y_0(\mathbf{I} + k_0^{-2}\Delta_\perp)^{-0.5}(\mathbf{I} - k_0^{-2}\nabla_\perp \times \nabla_\perp \times)$
- Lowest order approximation of exact IBC
  - $\boldsymbol{\Upsilon} \coloneqq Y_0\mathbf{I}$
  - 0th-order open BC (OBC0)
- Lowest order approximation of square root operator
  - $\boldsymbol{\Upsilon} \coloneqq pY_0(\mathbf{I} - k_0^{-2}\nabla_\perp \times \nabla_\perp \times)$
  - Choose p to optimize DDM-convergence rate
  - 0th-order open BC with curl-curl term (OBC0c)



ABSORBING BOUNDARY CONDITIONS
MODAL

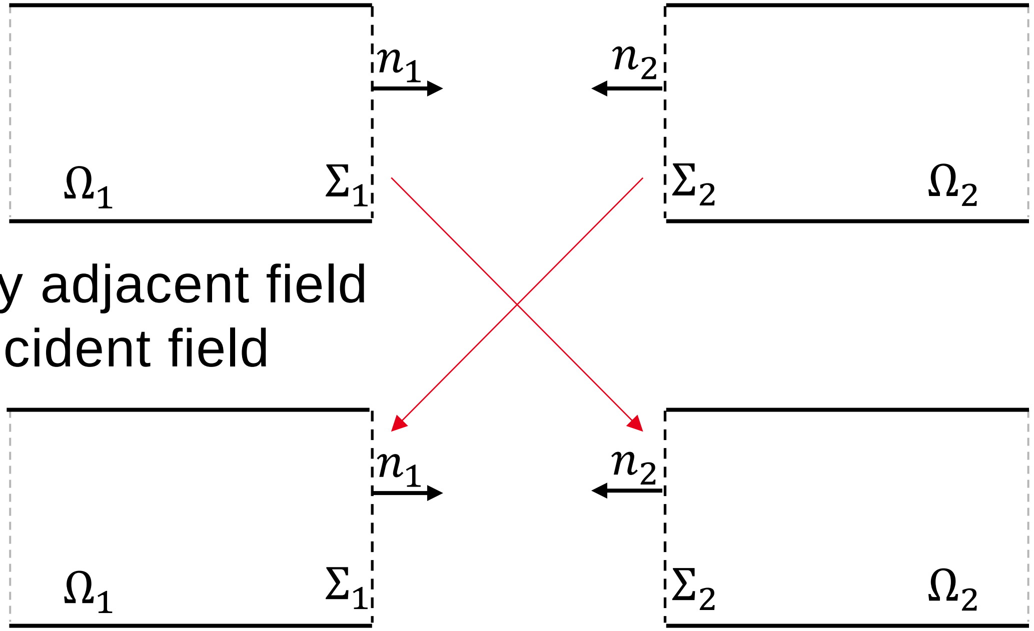
- Idea: describe outgoing waves by waveguide modes
- Representation of admittance operator
  - $\boldsymbol{Y}\gamma^{\mathrm{T}}(E) \coloneqq \sum_{m=1}^{\infty} Y_m(\omega) a_m(E) e_{\perp,m}$
  - Orthogonal terms
  - Admittances only depend on frequency
  - Exact for guided wave structures
  - Modal boundary condition (MBC)



- $a_m(E) = \int_{\Sigma_{\mathrm{ABC}}} \gamma^{\mathrm{T}}(E) \cdot e_m \,\mathrm{d}S$
- $Y_m^{\mathrm{TX}}(\omega) = \begin{cases} k_{\mathrm{n}}/\omega\mu & \text{for TE modes} \\ \omega\varepsilon/k_{\mathrm{n}} & \text{for TM modes} \\ Y_0 & \text{for TEM modes} \end{cases}$
- $k_n = \sqrt{k_0^2 - k_{n,\perp}^2}$

DOMAIN DECOMPOSITION
DOMAIN COUPLING

- Solve both subdomains with absorbing BC



- Apply adjacent field as incident field
- Solve again with new incident field

Solve:

Iteration count

- BVP 1 with $\gamma_1^{\mathrm{t}}(H_1^1) + \boldsymbol{\Upsilon}\gamma_1^{\mathrm{T}}(E_1^1) = 0$
- BVP 2 with $\gamma_2^{\mathrm{t}}(H_2^1) + \boldsymbol{\Upsilon}\gamma_2^{\mathrm{T}}(E_2^1) = 0$

Domain index

- BVP 1 with $\gamma_1^{\mathrm{t}}(H_1^2) + \boldsymbol{\Upsilon}\gamma_1^{\mathrm{T}}(E_1^2) = -\gamma_2^{\mathrm{t}}(H_2^1) + \boldsymbol{\Upsilon}\gamma_2^{\mathrm{T}}(E_2^1)$
- BVP 2 with $\gamma_2^{\mathrm{t}}(H_2^2) + \boldsymbol{\Upsilon}\gamma_2^{\mathrm{T}}(E_2^2) = -\gamma_1^{\mathrm{t}}(H_1^1) + \boldsymbol{\Upsilon}\gamma_1^{\mathrm{T}}(E_1^1)$

DOMAIN DECOMPOSITION
DOMAIN COUPLING

- General transmission condition (TC)
  - $\boldsymbol{\Upsilon}\gamma_i^{\mathrm{T}}(E_i) + \gamma_i^{\mathrm{t}}(H_i) = \boldsymbol{\Upsilon}\gamma_j^{\mathrm{T}}(E_j) - \gamma_j^{\mathrm{t}}(H_j)$
- Insertion of the admittance operators defines the specific TCs
  - Established
    - OTC0: $\boldsymbol{\Upsilon}\gamma^{\mathrm{T}}(E) \coloneqq Y_0\gamma^{\mathrm{T}}(E)$
    - OTC0c: $\boldsymbol{\Upsilon}\gamma^{\mathrm{T}}(E) \coloneqq pY_0(\mathbf{I} - k_0^{-2}\nabla_\perp \times \nabla_\perp \times)\gamma^{\mathrm{T}}(E)$
  - New
    - MTC: $\boldsymbol{\Upsilon}\gamma^{\mathrm{T}}(E) \coloneqq \sum_{m=1}^{\infty} a_m^{\mathrm{TX}}(E)Y_m(\omega)\, e_{\perp,m}^{\mathrm{TX}}$

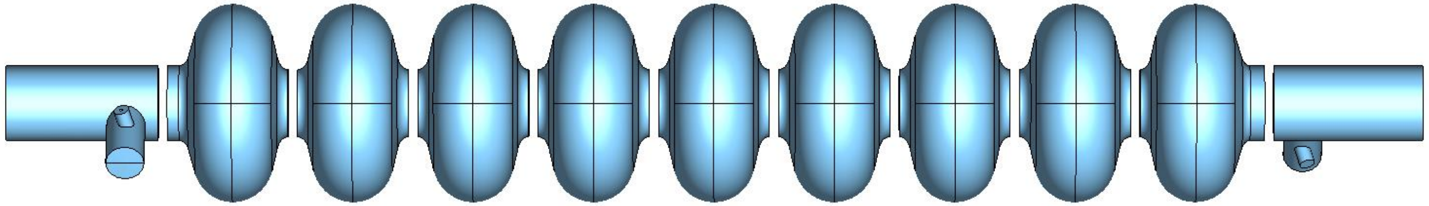
DOMAIN DECOMPOSITION
WEAK FORMULATION

- Weak formulation per subdomain: find $E \in H(\mathrm{curl})$ such that $\forall v \in H(\mathrm{curl})$:

$$\int_{\Omega_i} \mu^{-1}\, \nabla \times E \cdot \nabla \times v \,\mathrm{d}V - \omega^2 \int_{\Omega_\mathrm{i}} \varepsilon\, E \cdot v \,\mathrm{d}V =$$

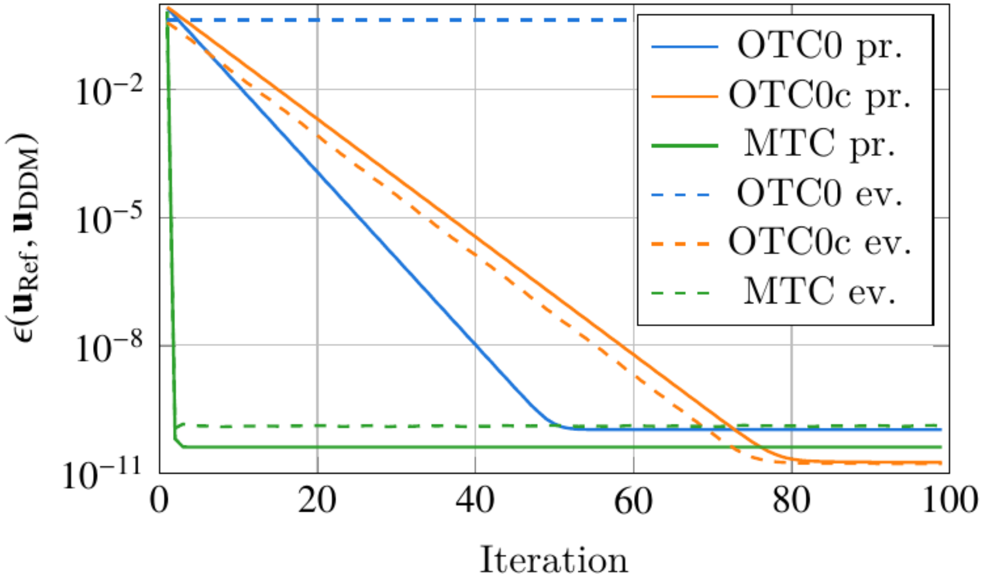
$$\underbrace{-j\omega \int_{\Omega_\mathrm{i}} J \cdot v \,\mathrm{d}V}_{\text{Current excitation}} - \underbrace{\int_{\Sigma_\mathrm{SI}} \mu^{-1}\gamma^\mathrm{t}(\nabla \times E) \cdot v \,\mathrm{d}S}_{\text{Resistive wall}} - \underbrace{\int_{\Sigma_\mathrm{WG}} \mu^{-1}\gamma^\mathrm{t}(\nabla \times E) \cdot v \,\mathrm{d}S}_{\text{Waveguides}} - \underbrace{\int_{\Sigma_\mathrm{DDM}} \mu^{-1}\gamma^\mathrm{t}(\nabla \times E) \cdot v \,\mathrm{d}S}_{\text{DDM interface}}$$

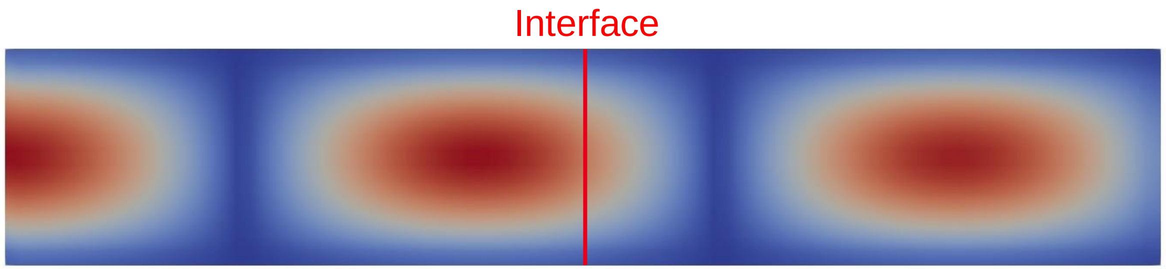
- Resistive wall BC: $\mu^{-1}\gamma^\mathrm{t}(\nabla \times E) = \mathrm{j}\omega Y(\omega)\gamma^\mathrm{T}(E)$
- Waveguide BC: $\mu^{-1}\gamma^\mathrm{t}(\nabla \times E) = \mu^{-1}\gamma^\mathrm{t}(\nabla \times E^\mathrm{Inc}) - j\omega \sum_{m=1}^{\infty} Y_m^\mathrm{TX}(\omega) a_m(E - E^\mathrm{Inc})\, e_{m,\perp}^\mathrm{TX})$



CONVERGENCE ON MODEL PROBLEMS
HOMOGENEOUS WAVEGUIDE

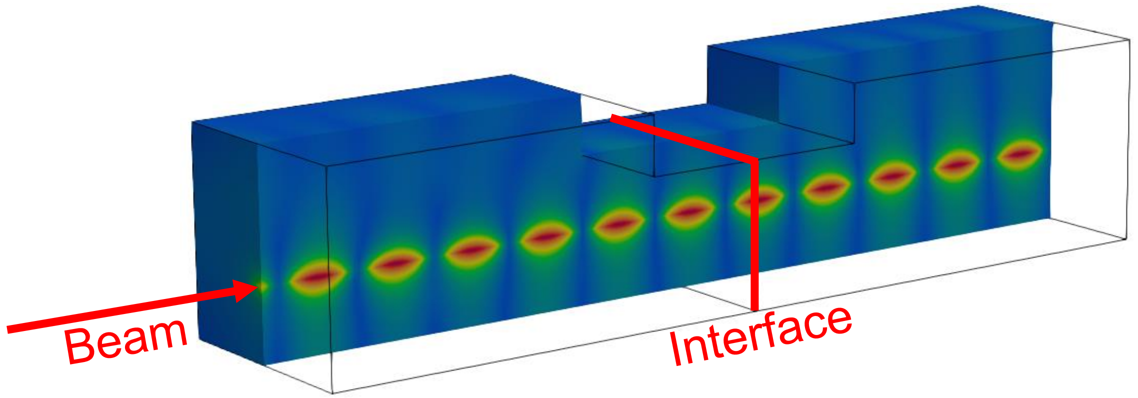
- Convergence histories of DDM with different TCs on homogeneous waveguide
- Convergence for OTC0 only in propagating case
- Convergence for OTC0c in both evanescent and propagating case
- Both OTCs lead to convergence factors $\gg 0$
- Convergence with MTC in one iteration





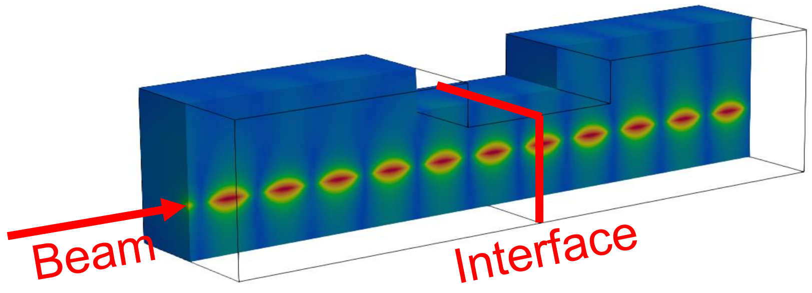
CONVERGENCE ON MODEL PROBLEMS
WAVEGUIDE TRANSITION

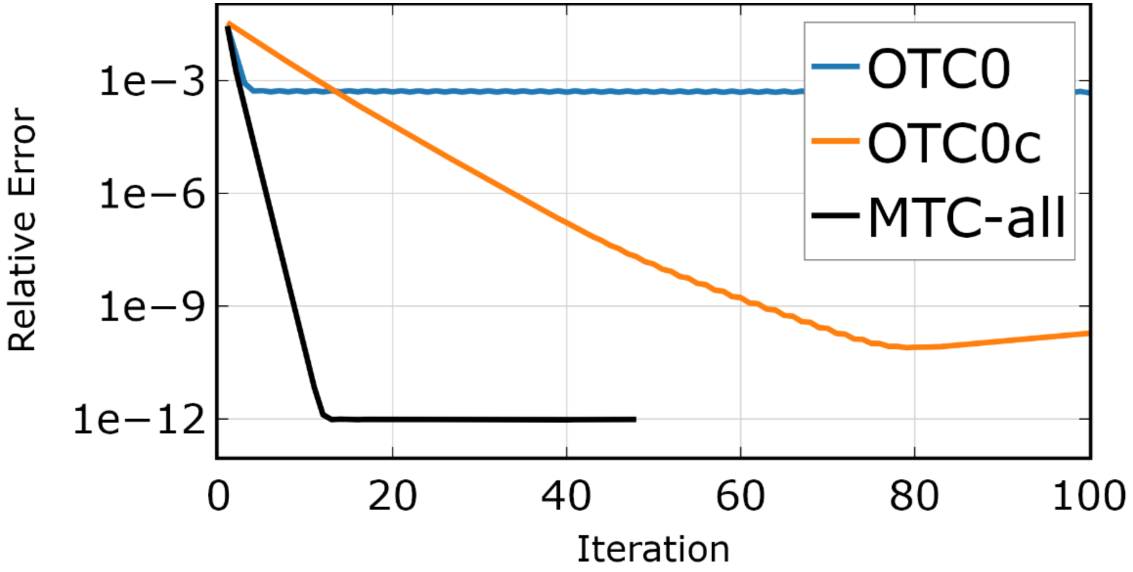
- Waveguide transition
  - 17.5 cm by 20 cm at entry and exit
  - 12.5 cm by 20 cm in the middle
- Beam excitation
  - $f = 2.1\ \mathrm{GHz}$
  - 2 TM and 5 TE modes propagate at the interface
  - Several modes on interface excited



CONVERGENCE ON MODEL PROBLEMS
WAVEGUIDE TRANSITION

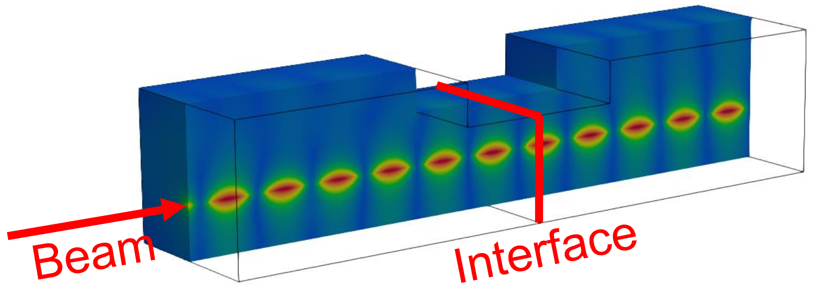
- OTC0
  - No convergence for evanescent modes
  - Insufficient accuracy
- OTC0c
  - Initially convergent at slow rate
  - Diverges at high iteration counts due to reflections of propagating modes
- MTC
  - Rapid convergence to machine precision
  - Large number of WG modes on interface
  - $\Upsilon\gamma^{\mathrm{T}}(E) \coloneqq \sum_{m=1}^{\infty} y_m(\omega) a_m(E) e_{\perp,m}$

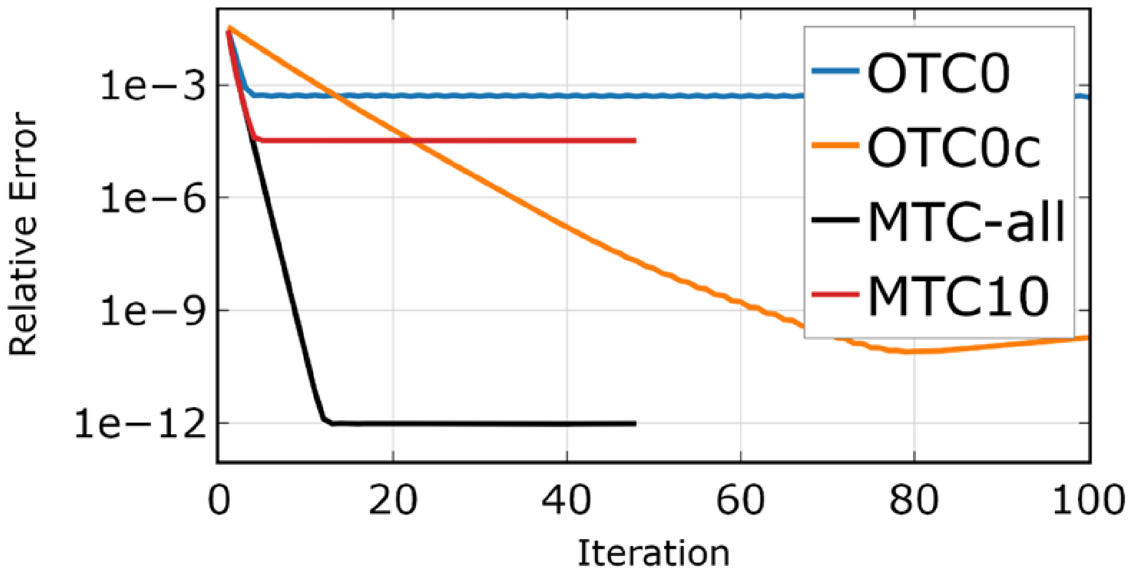




CONVERGENCE ON MODEL PROBLEMS
WAVEGUIDE TRANSITION

- MTC10
  - $\Upsilon\gamma^{\mathrm{T}}(E) := \sum_{m=1}^{M} y_m(\omega) a_m(E) e_{\perp,m}$
  - Truncate sum at small number of WG modes (e.g. 10 TE+10 TM)
  - Convergence only to limited accuracy



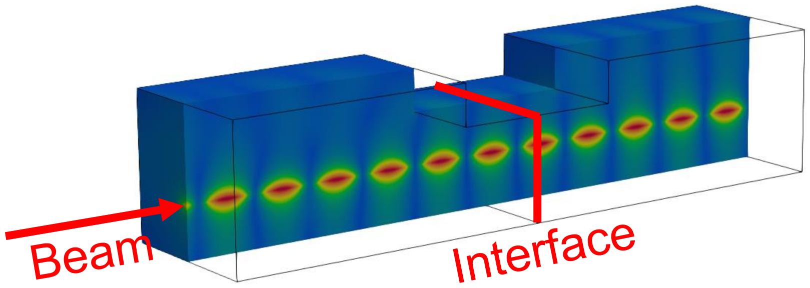


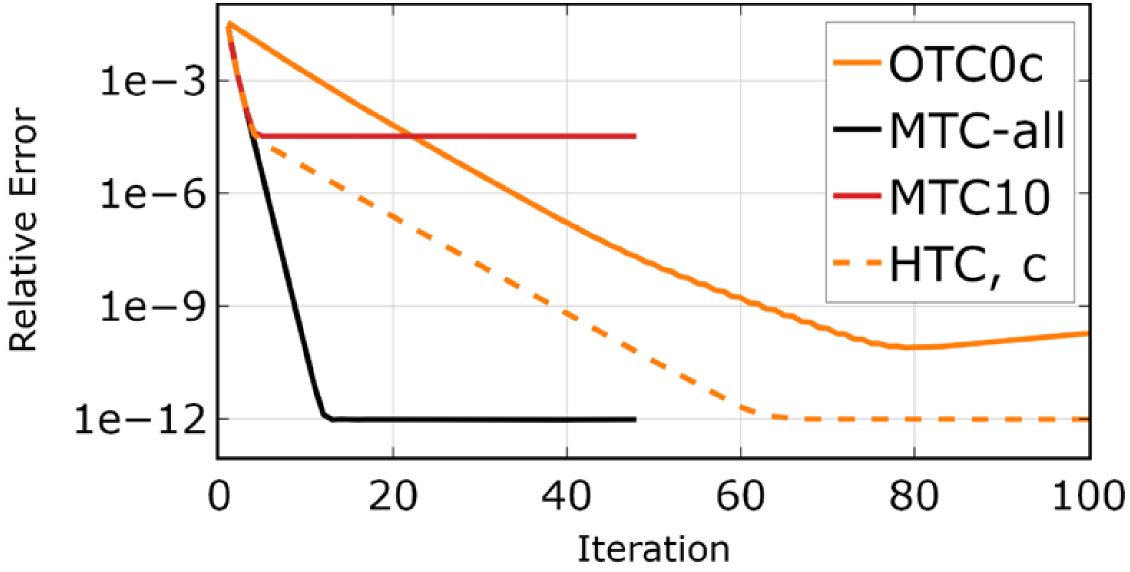
HYBRID TRANSMISSION CONDITION

- Idea: combine OTC and MTC
  - OTC: $\boldsymbol{\Upsilon}\gamma^{\mathrm{T}}(E) \coloneqq \boldsymbol{\Upsilon}^{\mathrm{OTC}}\gamma^{\mathrm{T}}(E)$
  - MTC: $\boldsymbol{\Upsilon}\gamma^{\mathrm{T}}(E) \coloneqq \sum_{m=1}^{\infty} a_m^{\mathrm{TX}}(E) Y_m(\omega)\, e_{\perp,m}^{\mathrm{TX}}$
  - HTC: $\boldsymbol{\Upsilon}\gamma^{\mathrm{T}}(E) \coloneqq \sum_{m=1}^{M} a_m^{\mathrm{TX}}(E)\left(Y_m(\omega)\boldsymbol{I} - \boldsymbol{\Upsilon}^{\mathrm{OTC}}\right) e_{\perp,m}^{\mathrm{TX}} + \boldsymbol{\Upsilon}^{\mathrm{OTC}}\gamma^{\mathrm{T}}(E)$
    - Convergent method
    - Only small number of modes must be considered explicitly

CONVERGENCE ON MODEL PROBLEMS
WAVEGUIDE TRANSITION

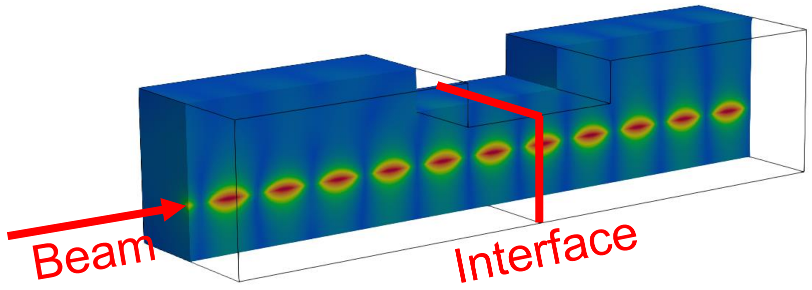
- HTC
  - MTC10+OTC0c with complex p
  - Rapid initial convergence of MTC
  - Asymptotic convergence rate as for evanescent modes of OTC0c
  - Propagating modes are represented exactly by the MTC
    $\Longrightarrow$ Convergence to machine precision

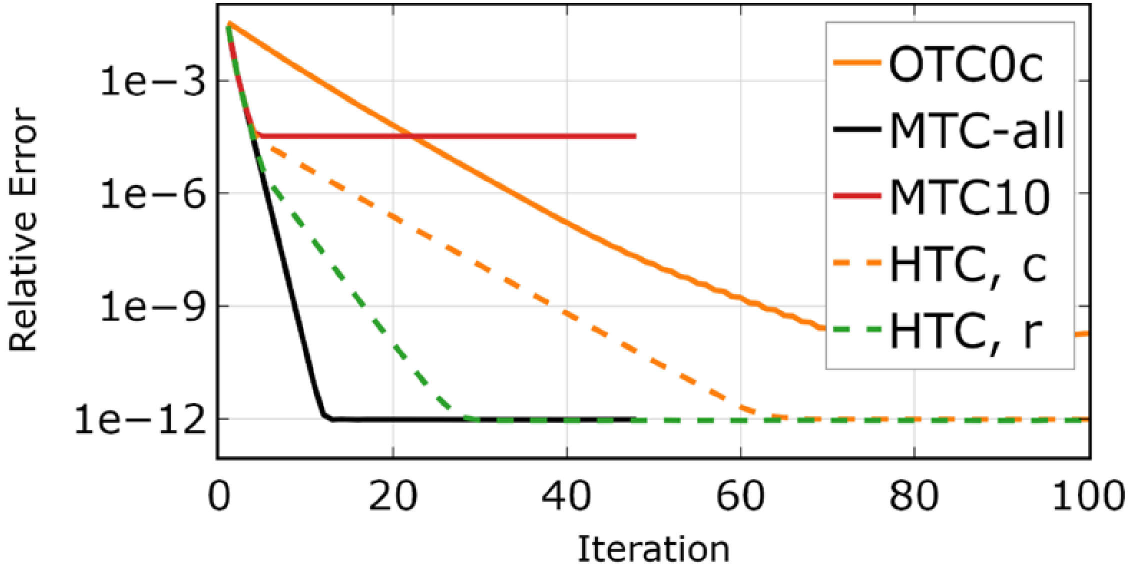




CONVERGENCE ON MODEL PROBLEMS
WAVEGUIDE TRANSITION

- HTC
  - MTC10+OTC0c with complex p
  - Rapid initial convergence of MTC
  - Asymptotic convergence rate as for evanescent modes of OTC0c
  - Propagating modes are represented exactly by the MTC
    $\Longrightarrow$ Convergence to machine precision
- Optimize p only for remaining evanescent modes
  - Significantly improved convergence

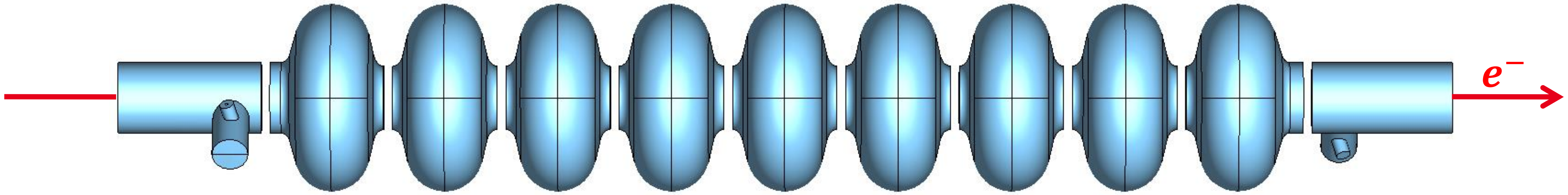




TESLA CAVITY

- Computation of beam impedance
- Beam impedance: $Z = \frac{1}{I_0^2} \int_\Omega J^* \cdot E \, \mathrm{d}V$
- PEC boundary
- Truncated modal BC for beam pipes and couplers

- Finite elemtent discretization
- 411 000 elements, 2nd order basis functions
- 6.2 million DoF
- 11-domain decomposition
- GMRES iteration scheme
- Convergence criterion: GMRES residual=1e-6



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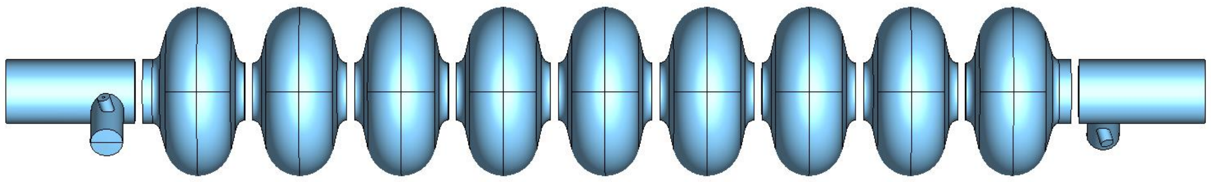
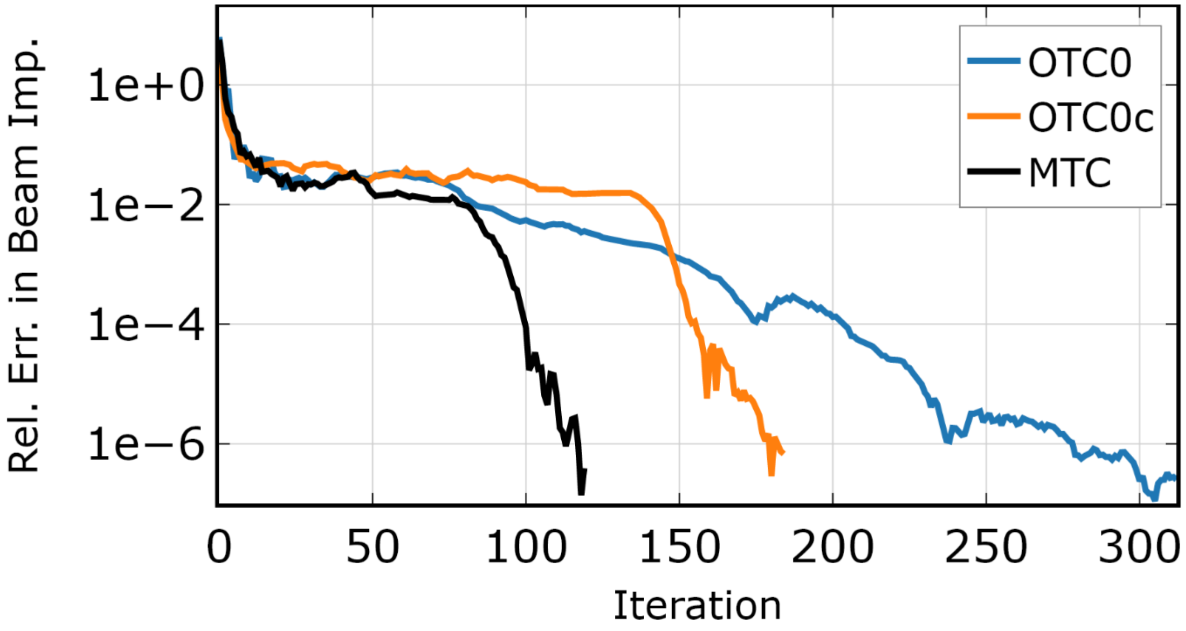
TESLA CAVITY
IMPEDANCE COMPUTATION AT 5 GHZ

- MTC leads to significantly faster convergence than both OTCs
- Large number of modes on interfaces (≈ 4200) for MTC





- 411 000 elements, 2nd order basis functions
- 6.2 million DoF
- 11-domain decomposition
- GMRES iteration scheme, f=5.0 GHz
- Conv. criterion: GMRES residual=1e-6

TESLA CAVITY

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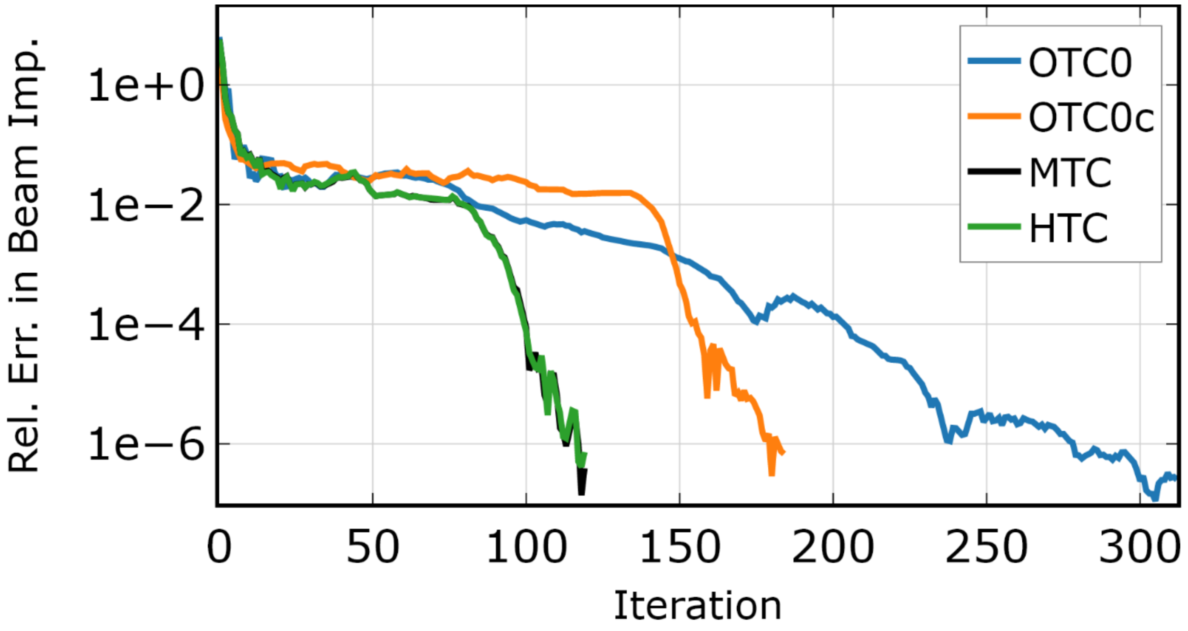

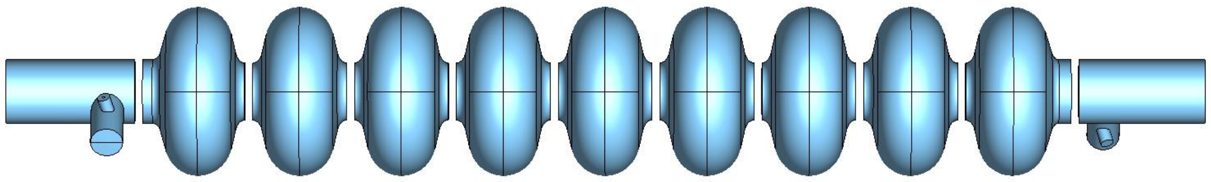

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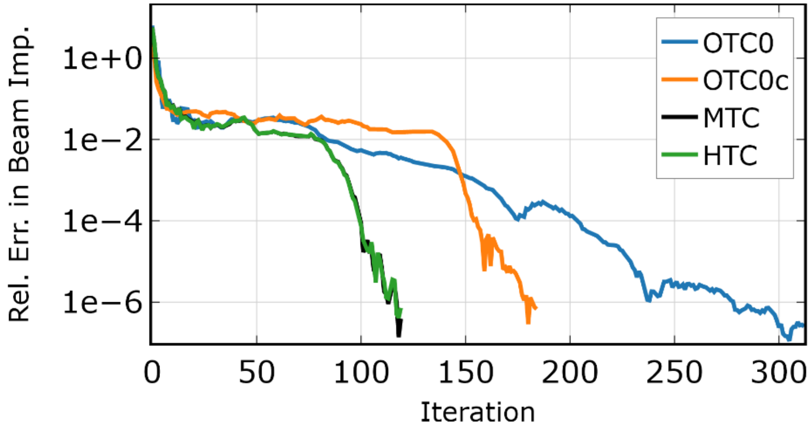
- 11-domain decomposition
- GMRES iteration scheme, f=5.0 GHz
- Conv. criterion: GMRES residual=1e-6

- HTC with 100 TE and 100 TM modes
  - Leads to almost identical performance as MTC
- $\approx 30\%$ reduction of iterations compared to OTC0c

TESLA CAVITY
IMPEDANCE COMPUTATION AT 5 GHZ

- Runtime measurement on **Lichtenberg HPC with 11 nodes** for single frequency
- MTC leads to
  - Significant improvement of cost in DDM iterations
  - Significant overhead in update matrix step

TC	Update Matrix	Cholesky	DDM Iterations	total
OTC0	6s	36s	891s	933s
OTC0c	**7s**	36s	**522s**	565s
MTC	**105s**	38s	**363s**	506s
HTC100	13s	37s	358s	408s



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TESLA CAVITY
IMPEDANCE COMPUTATION AT 5 GHZ

- Runtime measurement on **Lichtenberg HPC with 11 nodes** for single frequency
- HTC with 100 TE and 100 TM modes leads to
  - Minor difference in cost of iteration phase compared to MTC
  - Significant improvement (28%) of total cost compared to OTC0c

TC	Update Matrix	Cholesky	DDM Iterations	total
OTC0	6s	36s	891s	933s
OTC0c	**7s**	36s	522s	**565s**
MTC	105s	38s	363s	506s
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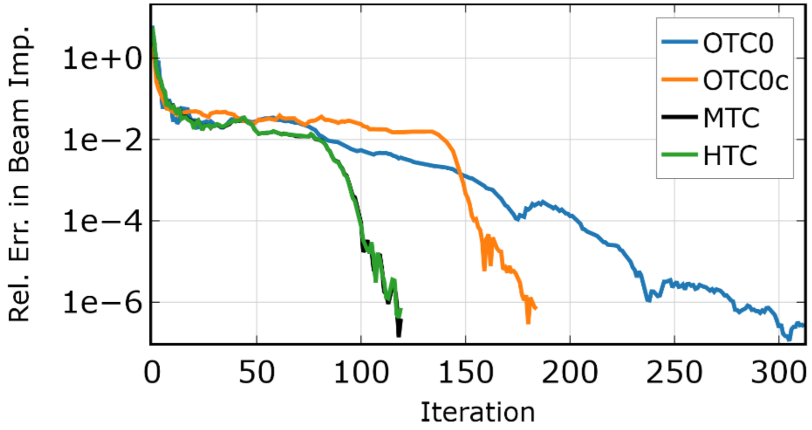
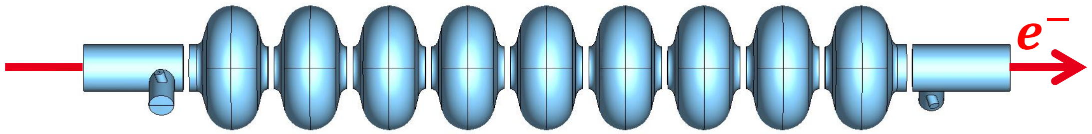


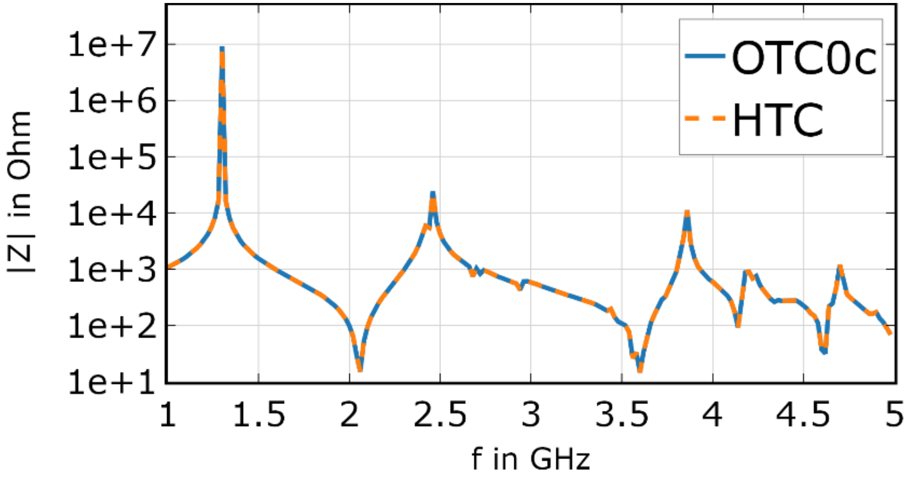
- 411 000 elements, 2nd order basis functions
- 6.2 million DoF
- 11-domain decomposition
- GMRES iteration scheme, f=5.0 GHz
- Conv. criterion: GMRES residual=1e-6

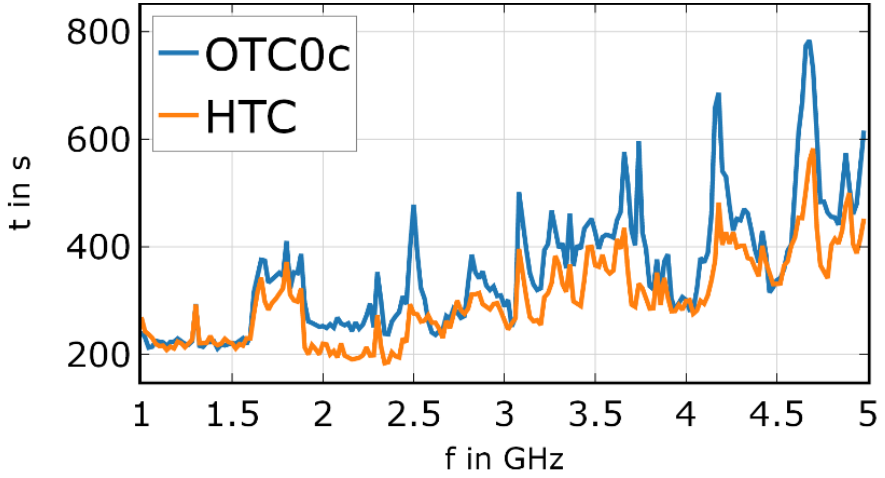
TESLA CAVITY
BROADBAND IMPEDANCE COMPUTATION

- TESLA cavity 1-5 GHz
- GMRES residual: 1e-8
- Excellent agreement between both methods

- DDM with HTC almost consistently faster
- 15% overall reduction in computational cost

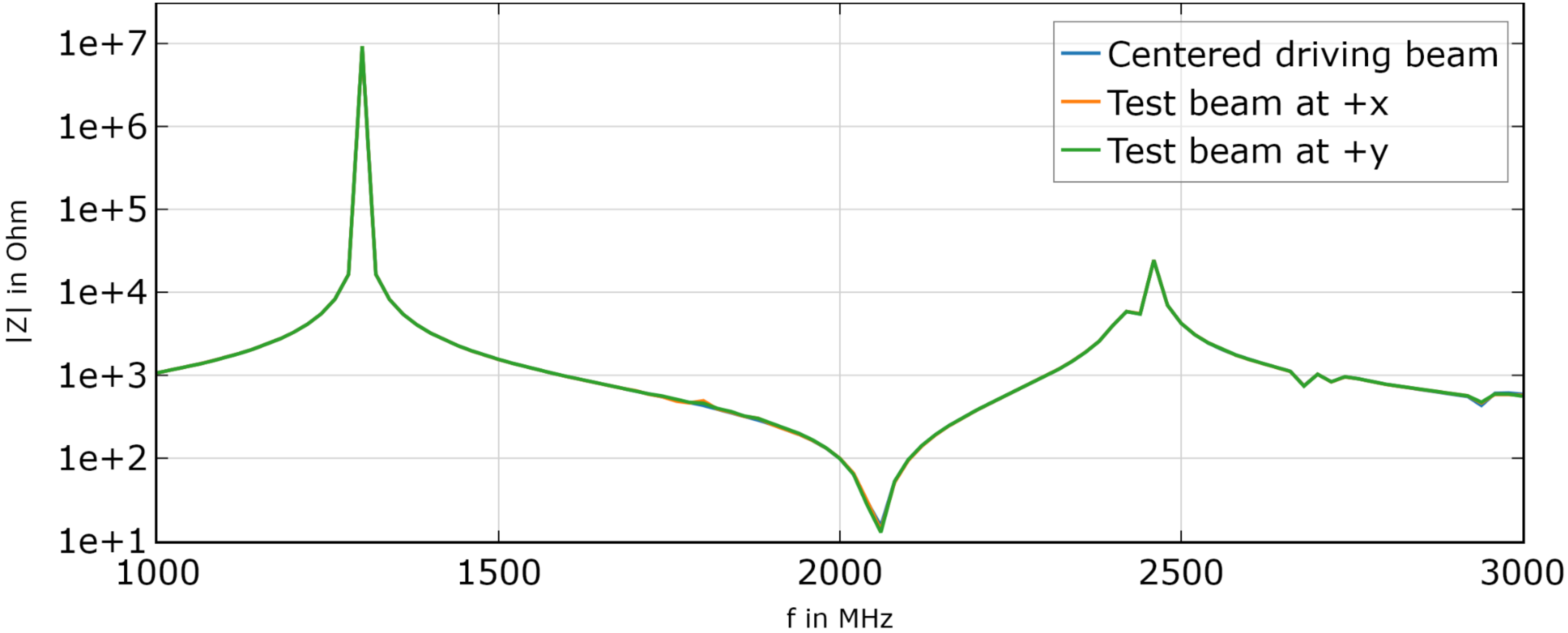


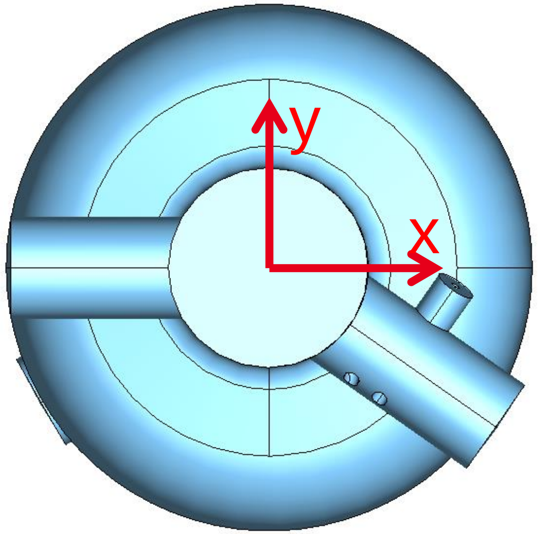




TESLA CAVITY
BROADBAND IMPEDANCE COMPUTATION

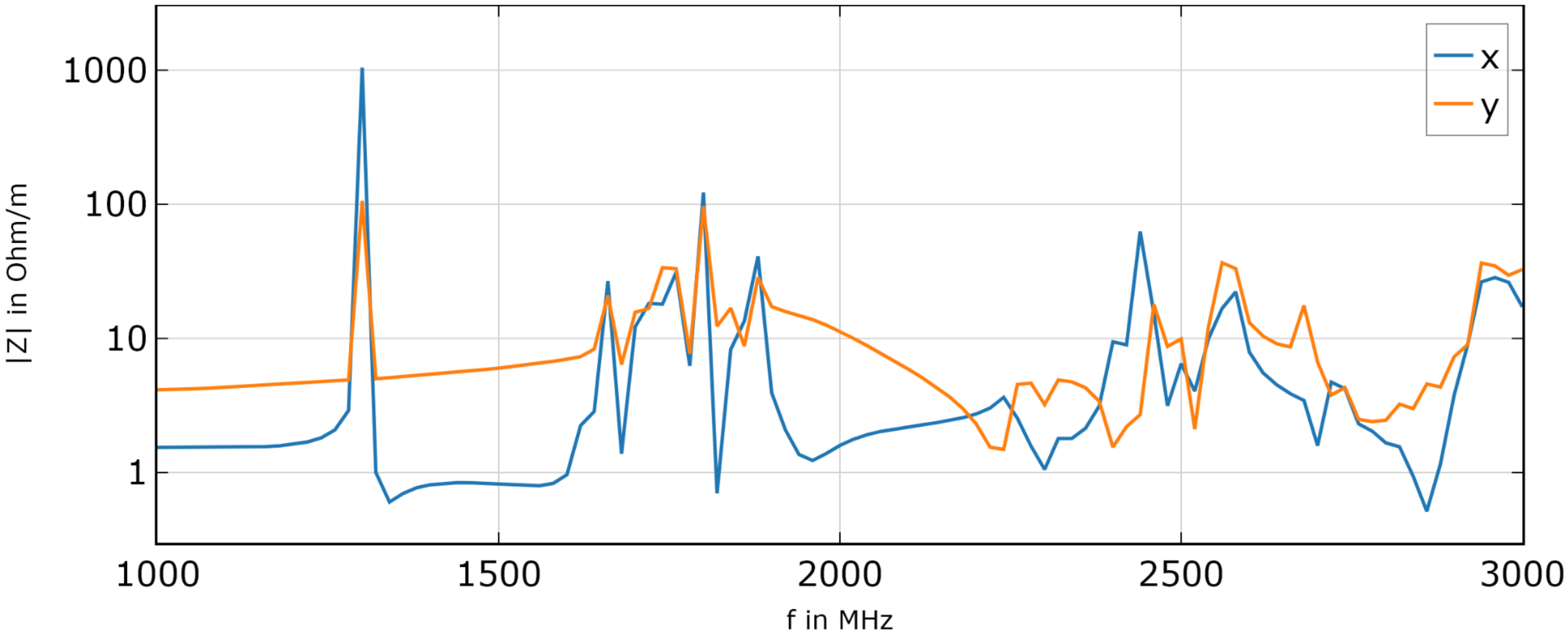
- Longitudinal impedance for displaced test beams
- Minor impact of displacement

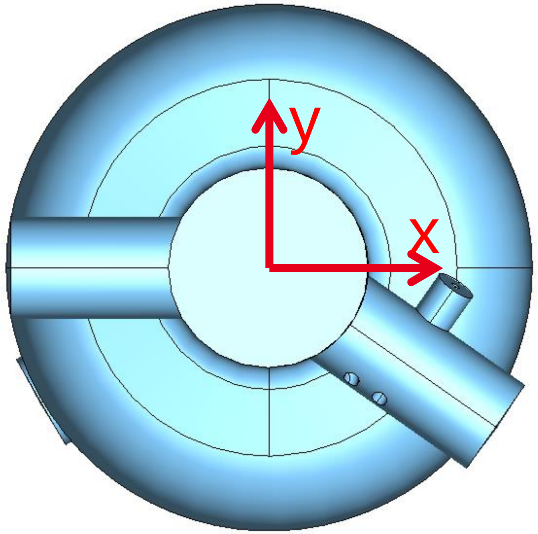




TESLA CAVITY
BROADBAND IMPEDANCE COMPUTATION

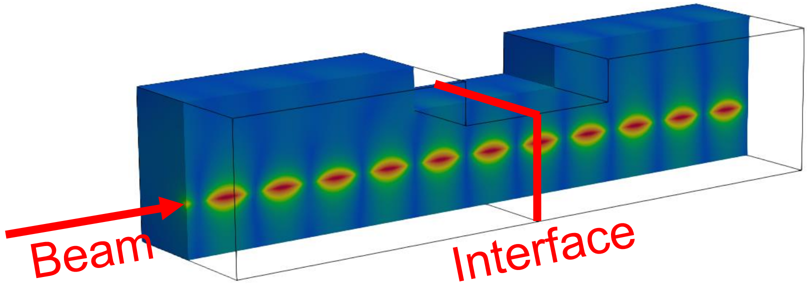
- Transverse impedance for displaced test beams
- Impedance at 1.3 Ghz mainly in x-direction
  - Likely due to main coupler
- Comparably large transverse impedances between 1.5 and 2 GHz

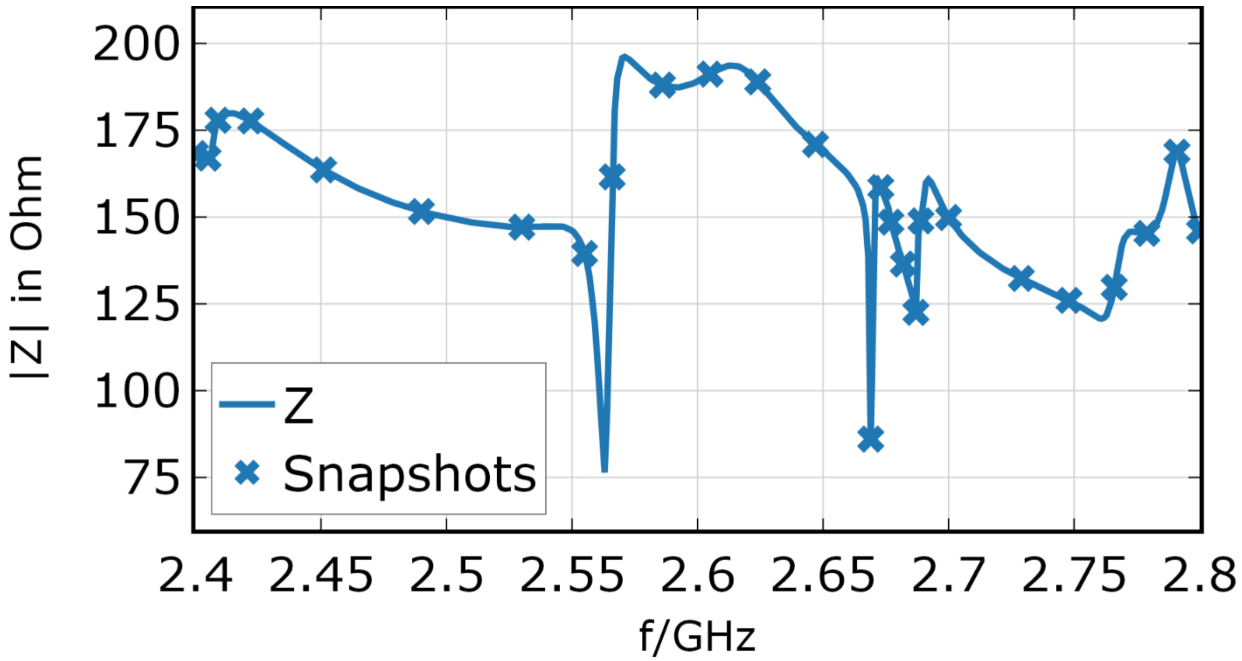




UPDATE ON FAST FREQUENCY SWEEP

- Implemented FFS based on RBM (MOR) for DDM
- Adaptive sampling
  - New sample at frequency with largest error
  - Efficient distribution and minimal number of samples
  - Overhead for error estimation <10% for large problems
- MPI-parallel implementation
- Work in progress
  - Currently only for two domains





CONCLUSION

- Introduced two new transmission conditions for Schwarz DDM
  - Modal transmission condition (MTC)
  - Hybrid transmission condition (HTC)
- MTC leads to optimal convergence on the waveguide problem
- Both new TCs improve convergence rate and stability of the DDM
- Application to the TESLA cavity on Lichtenberg HPC
  - Improvements verified with large scale problem
- Update on the FFS