

3D Electromagnetic Time-Domain wake and impedance solver

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Outline

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| 1. Introduction to Beam-Coupling Impedance simulations |
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| 2. wakis code framework and architecture |
| 3. The Finite Integration Technique (FIT): |
| 3.1. Numerical Algorithm in free-space |
| 3.2. Geometry definition: STL importer |
| 3.3. Materials ε , μ , σ and EM sources |
| 3.4. Wake potential and impedance |
| 3.5. Low- β simulations |
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4. Conclusions, Present & Future work

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Beam-coupling impedance

- Electromagnetic wakefields are generated as the particle beam traverses the different accelerator devices with discontinuities in the geometry (cavities, transitions...) or the electromagnetic properties (ε, μ, σ). These wakefields will affect the trailing particles/bunches and can generate instabilities
- The beam-coupling impedance **Z** is a frequency-dependent property of each accelerator device, used to quantify the wakefields' effects

$$\mathbf{Z}_{||}(\omega) = -\frac{\int_{-\infty}^{\infty} W_{||}(s) e^{-i\omega s} ds}{\int_{-\infty}^{\infty} \beta c \lambda(s) e^{-i\omega s} ds}$$



Importance of beam-coupling impedance



The impedance of all relevant accelerator components is gathered in each accelerator's impedance model





Beam stability

And used in beam-dynamics codes (e.g., pyHeadtail, Xsuite) to predict beam behaviour and stability

Beam induced heating

Assess beam-induced heating of individual accelerator components and propose mitigation solutions



How to compute beam-coupling impedance?

Analytical calculations

Beam-coupling impedance can be derived analytically for simple geometries and material configurations^[4]:

e.g., cylindrical pillbox cavities, pipe transitions, single-layer resistive wall

Numerical computations

For more complex accelerator devices, the numerical solution of Maxwell's equations in frequency or time-domain is required.

- \circ In frequency domain:
 - 2D models for vacuum chamber multi-layered elements e.g., ImpedanceWake2D^[5]
 - Commercial CST[®] Eigenmode solver → loss-less resonant modes of general 3D structures without excitation + impedance in post-processing

\circ In time-domain:

- Time-domain allows for full-wave electromagnetic simulations including losses and excitation bunch. Several codes available following different approaches e.g.:
 - ABCI (axi-symmetric), CST[®] Wakefield solver (3D), GdfidL[®], PBCI, ECHO-3D (3D, moving window) → not on an open-source platform



[4] Wake fields and impedance, L. Palumbo, V.G. Vaccaro, CERN-1995-006.331



[5] ImpedanceWake2D, N. Mounet, TUO1C02 HB'10 https://gitlab.cern.ch/IRIS/IW2D

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About the project:

Project start:

wakis as post-processing tool

Computation of wake potential and impedance from **pre-computed fields** from other EM solvers

Longitudinal $Z_{||}$ and transverse Z_{\perp} (dipolar & quadrupolar) successfully benchmarked with CST[®] fields

2022

Towards open-source Wakefield solver:

Coupling post-processing wakis with open-source PIC-EM solver WarpX^[6]

Successfully benchmarked lossless pillbox cavity below cutoff^[7]

> Don't reinvent the wheel !

2023

Exploring FIT mock-up in Python

Implementing the Finite Integration Technique (FIT) fully in Python to explore computational viability and benefit from the open-source community Present:

wakis as an open-source 3D time-domain electromagnetic wake and impedance solver as the foundation to address computational challenges

[6] ECP-WarpX: <u>https://ecp-warpx.github.io/</u>[7] E. de la Fuente, WEPL170 IPAC'23



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Available on GitHub

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| | elenafuengar adding 3d plot | https://github.com/ImpedanCEI/wakis | 423e8ca · 1 hour ago 🕚 382 Commits | 3D electromagnetic time-domain solver, specialized in wake potential and beam- |
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Documentation on ReadTheDocs



* » *P* Overview C Edit on GitHub Welcome to wakis documentation wakis: 3D Time-domain Wake and Impedance Solver wakis is a 3D Time-domain Electromagnetic solver that solves the Integral form of Maxwell's equations using the Finite Integration Technique (FIT) numerical method. It computes the longitudinal and transverse wake potential and beam-coupling impedance from the simulated electric and magnetic fields. It is hence focused on simulations for particle accelerator components, but it is also a multi-purpose solver; capable of simulating planewaves interaction with nanostructures, optical diffraction, and much more! Some of wakis features: • Material tensors: permittivity ε , permeability μ , conductivity σ . Possibility of anisotropy. CAD geometry importer (.stl format) for definition of embedded boundaries and material regions, based on pyvista Boundary conditions: PEC, PMC, Periodic, ABC-FOEXTRAP Different time-domain sources: particle beam, planewave, gaussian wavepacket • 100% python, fully exposed API (material tensors, fields E, H, J). Matrix operators based on numpy and scipy.sparse routines ensure fast calculations. 1d, 2d, 3d built-in plotting on-the-fly Optimized memory consumption GPU acceleration using cupy/cupyx Perfect matching layer (PML) coming soon! The source code is available in the wakis GitHub repository.

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wakis solver architecture





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Examples & benchmarks

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Finite Integration Technique

Maxwell Equations (Integral form)

$$\oint_{\partial A} E \cdot ds = -\iint_{A} \frac{\partial B}{\partial t} \cdot dA$$

$$\oint_{\partial A} H \cdot ds = -\iint_{A} \left(\frac{\partial D}{\partial t} + J\right) \cdot dA$$

$$\oint_{\partial V} B \cdot dA = 0$$

$$\oint_{\partial V} D \cdot dA = \iiint_{V} \rho \, dV$$

$$D = \varepsilon E$$
, $B = \mu H$, $J = \sigma E + \rho v$

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 1^{st} approximation Domain discretization dx, dy, dz



Maxwell Grid Equations

 $CD_{s}e = -D_{A}\frac{\partial b}{\partial t}$ $\widetilde{C}\widetilde{D}_{s}h = \widetilde{D}_{A}\left(\frac{\partial d}{\partial t} + j\right)$ $SD_{A}b = 0$ $\widetilde{S}\widetilde{D}_{A}\left(\frac{\partial d}{\partial t} + j\right) = 0$ $d = \widetilde{D}_{\varepsilon}e, \quad b = D_{\mu}h, \quad j = \widetilde{D}_{\sigma}e + j_{src}$

- Operators
- Grid areas and lengths
- Materials

Finite Integration Technique (II)



Finite Integration Technique (III)

$$h^{n+1} = h^n - \Delta t \, \widetilde{D}_s D_{\mu}^{-1} D_A^{-1} C e^{n+0.5}$$
$$e^{n+1.5} = e^{n+0.5} + \Delta t D_s \widetilde{D}_{\varepsilon}^{-1} \widetilde{D}_A^{-1} \widetilde{C} h^n - \widetilde{D}_{\varepsilon}^{-1} j_{src}^n$$
$$- \widetilde{D}_{\varepsilon}^{-1} \widetilde{D}_{\sigma} e^{n+0.5}$$



- C, C Curl operator: [3N_{cell} x 3N_{cell}] sparse matrix that relates the E and H fields and defines PEC, PMC or Periodic boundary conditions (BCs)
- $\circ \quad D_A, D_s, \widetilde{D}_A, \widetilde{D}_s: 3N_{cell} \text{ diagonal matrices} \\ \text{ containing the grid (primal and dual)} \\ \text{ discretization in terms of cell lengths} \\ \text{ and areas}$





 $\circ e^{n+1.5}, h^{n+1}, j^n$ Fields: saved in memory as $[3N_{cell}]$ lexicographic arrays, updated every simulation timestep.

Fully-exposed, modifications on-the-fly (e.g. addition of **sources or initial conditions**)



Stipy.sparse Materials $D_{\varepsilon}^{-1}, D_{\mu}^{-1}, D_{\sigma}$

- $\widetilde{D}_{\varepsilon}^{-1}$, D_{μ}^{-1} : 3N_{cell} diagonal matrices for the anisotropic inverse permittivity ε and permeability μ rank-2 tensors
- \tilde{D}_{σ} : 3N_{cell} diagonal matrix for the anisotropic electric conductivity rank-2 tensor. The current can be computed as: $j^{n+1} = \tilde{D}_{\sigma} e^{n+0.5} + j^n_{src}$

Importing CAD geometry and visualization

PyVista

3D plotting and mesh analysis through a streamlined interface for the Visualization Toolkit (VTK)



https://github.com/pyvista/pyvista

EAbs field, timestep=630



Using **PyVista** capabilities, wakis can:

- o Import CAD geometry: geometry = pv.read(CAD_file)
- Generate the domain grid: grid = pv.StructuredGrid(X, Y, Z) and find the domain cells inside the CAD solids with optimized collision filters
- Assign material properties to each cell inside solid and subpixel smoothing to mitigate corner artifacts
- State-of-the-art interactive 3d plotting

Example: importing the LHC TCPC Crystal goniometer CAD file



Example: wakis interactive
grid.inspect() method



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Simulations with materials and sources

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Simulations with materials and sources (II)





Wake potential and impedance

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Wake potential and impedance (II)

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Low- β simulations

Beam current source with β

$$J_{z}(x_{s}, y_{s}, z) = \frac{q\beta c}{\sqrt{2\pi\sigma_{z}}} e^{\frac{-(s-s_{0})^{2}}{2\sigma_{z}^{2}}}$$
$$s = z - \beta ct; \quad s_{0} = z_{min} - \beta ct$$

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Simulations with a non-ultra relativistic beam have proven challenging with current simulation tools due direct & indirect space charge effects \rightarrow finer mesh

Wakis imulations for relativistic β ∈ {0.4, 1} have been benchmarked with CST[®] Wakefield solver



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Low- β simulations (II)

Beam current source with β

$$J_{z}(x_{s}, y_{s}, z) = \frac{q\beta c}{\sqrt{2\pi\sigma_{z}}} e^{\frac{-(s-s_{0})^{2}}{2\sigma_{z}^{2}}}$$
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Simulations with a non-ultra relativistic beam have proven challenging with current simulation tools due direct & indirect space charge effects \rightarrow finer mesh

▶ Wakis simulations for relativistic $\beta \in \{0.4, 1\}$ have been benchmarked with CST[®] Wakefield solver

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Example 5: Comparison of W_{\parallel} and Z_{\parallel} for different values of beam β Benchmark with CST Wakefield Solver



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Conclusions

- Developed a **3D Electromagnetic and Wake Solver in time domain**, 100% in python, based on the Finite Integration Technique:
 - Based on numpy & scipy
- CAD geometry import
- BCs: PEC, PMC, Periodic, PML*
- Anisotropic materials ε , μ , σ
- State of the art 2d, 3d plotting
- Available on GitHub and PyPI

- EM Sources & beam current with β
- GPU accelerated
- Fully exposed API
- Documentation with Sphinx
- wakis solver has been benchmarked with CST Wakefield Solver[®]
 with pillbox cavities of different materials and geometries

 Stepping-stone towards a collaborative open-source electromagnetic & wakefield solver capable of addressing present and future Impedance challenges









Present & Future work

- The code is under continuous development and optimization to accommodate current impedance challenges: FCC-ee & CLIC impedance model, Muon collider ionization cooling studies,...
- Some present work includes:
 - o Optimization of the existing PML boundaries
 - Implementation of Shchukin-Leontovich condition for good conductors
 - Addition of dispersive materials
 - Multi-core parallelization with mpi4py
 - Student M. Raschke working on wake extrapolation of partially decayed wakes
- Some future work considers:
 - Exploring the implementation of co-moving window for short-range wakes
 - Improving grid discretization and mesh refinement
 - Correct numerical dispersion

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mpi4py

Thank you for the attention ③



Wakis: 3D Electromagnetic Time-Domain wake and impedance solver

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Simulation script example

\$ipython script.py



from wakis import GridFIT3D, SolverFIT3D, WakeSolver
import pyvista as pv

```
# ----- Domain and Grid setup ------
# Number of mesh cells
Nx = 57
Ny = 57
Nz = 109
#dt = 5.707829241e-12
# Geometry Import
stl cavity = 'cavity.stl'
stl pipe = 'beampipe.stl'
stl_solids = {'cavity': stl_cavity, 'pipe': stl_pipe}
# Materials
stl_materials = {'cavity': 'vacuum', 'pipe': 'vacuum'}
background = [1.0, 1.0, 100] # lossy metal [\varepsilon r, \mu r, \sigma]
# Domain bounds (from stl)
surf = pv.read(stl cavity) + pv.read(stl pipe)
xmin, xmax, ymin, ymax, zmin, zmax = surf.bounds
# Set grid and geometry
grid = GridFIT3D(xmin, xmax, ymin, ymax, zmin, zmax, Nx, Ny, Nz,
                stl solids=stl solids,
                stl materials=stl materials)
#grid.inspect()
```

| # Beam | source |
|---------------------|---|
| # Beam parameters a | nd wake obj. |
| beta = 0.8 | # beam relativistic beta |
| sigmaz = beta*6e-2 | <pre># [m] -> multiplied by beta to have f_max cte</pre> |
| q = 1e-9 | # [C] |
| xs = 0. | <pre># x source position [m]</pre> |
| ys = 0. | <pre># y source position [m]</pre> |
| xt = 0. | <pre># x test position [m]</pre> |
| yt = 0. | <pre># y test position [m]</pre> |
| # tinj = 8.53*sigma | <pre>z/(beta*c) # injection time offset [s]</pre> |

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A word on wake potential W(s)

Wake function w(s) cannot be obtained for distributed source of charge λ (i.e., a beam), but instead the **wake potential** W(s). For a beam traversing a device in the positive *z* direction:

$$W(x_{s}, y_{s}, x_{t}, y_{t}, s) = \frac{1}{q_{1}} \int_{-\infty}^{\infty} dz [E(x_{s}, y_{s}, x_{t}, y_{t}, z, t) + ce_{z} \times B(x_{s}, y_{s}, x_{t}, y_{t}, z, t)]_{t = \frac{(s+z)}{c}}$$

Where x_s , y_s is the transverse position of the source beam λ , and x_t , y_t is the transverse position of the integration path.

We can conveniently separate the **longitudinal plane** (\parallel) and the transverse plane (\perp), having:

$$W_{||}(x_{s}, y_{s}, x_{t}, y_{t}, s) = \frac{1}{q_{1}} \int_{-\infty}^{\infty} E_{Z}\left(x_{s}, y_{s}, x_{t}, y_{t}, z, t = \frac{(s+z)}{c}\right) dz$$

Using the **direct integration method**, we can obtain the longitudinal wake potential from the 4D (spatial + time) electric field data $E_z(x, y, z, t)$ by computing this integral



A word on Impedance Z(f)

Impedance Z(f) can be calculated from the wake potential W(s) (longitudinal and transverse) by the Fourier transform (FT) of the former divided by the FT of the charge distribution $\lambda(s)$:

To compute the FT, the scipy or numpy FFT algorithms are fast and reliable.

To match CST[®] single sided DFT, defined by [1]:

$$S(\omega) = \frac{\Delta t}{\sqrt{\pi}} \sum_{k=0}^{1000} s(k) e^{-ik\Delta t\omega}$$

We use np.fft.fft routine with:

- *i.* $f_{max} = \frac{c}{\pi \sigma_z}$ maximum frequency the beam excites
- ii. $\Delta f = \Delta s/c$ freq. resolution defined by timestep
- iii. Length N (for zero padding) $N = 1001/(\Delta f \cdot f_{max})$

```
[1] CST Studio<sup>®</sup> Wakefield Solver Overview [link]
```

```
# import charge distribution in z
load charge_dist
lambda = interpolate(s, z, charge_dist/q)
# or analytically
lambda =1/(\sigma_z \sqrt{pi})*exp(-(s**2)/(2*\sigma_z **2))
# calculate FFT
lambdaf = np.fft.fft(lambda*c, n=N)
WPf = np.fft.fft(WP*1e-12, n=N) #[pC]
f = np.fft.fftfreq(N, \Delta f)
# calculate impedance
Z = - WPf / lambdaf
```