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NEW ACE3P CAPABILITIES AND CODE INTEGRATION OF ACE3P WITH GEANT4 AND LUME

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Abstract

The Advanced Computational Electromagnetic 3D Parallel simulation suite (ACE3P), developed by SLAC National Accelerator Laboratory, is a state-of-the-art multi-physics toolkit designed for virtual prototyping of accelerator and RF components. Leveraging over two decades of development, ACE3P integrates advanced physics modeling, including thermal and structural modelling, capabilities with scalable numerical algorithms to deliver cutting-edge simulations. The suite, comprised of seven application modules, utilizes high-order curved finite element methods to achieve high accuracy while enabling fast simulations for large-scale problems.

Two recent advancements include the integration with Geant4, for radiation studies and positron source generation, and the development of LUME-ACE3P, built on the Python framework of the LUME project, which streamlines parameter sweeps and optimization tasks. Furthermore, other code developments are presented here including more LUME-ACE3P functionality, dispersive material applications, and dynamic mode decomposition analysis.

INTRODUCTION

The multi-physics software toolkit Advanced Computational Electromagnetic 3D Parallel (ACE3P) has been developed at SLAC and has seen numerous improvements and added features over many years [1]. A recent ACE3P code workshop hosted at SLAC has noted an increasing interest in robust and efficient electromagnetic (EM) computations on HPC resources, especially for workflow management and code integration [2]. A brief list and overview of the various ACE3P code modules is given here:

- Omega3P – frequency-domain eigenmode solver
- S3P – frequency-domain S-parameter solver
- T3P – time-domain transient and wakefield solver
- Track3P – particle trajectory solver for multipacting
- Pic3P – particle-in-cell beam and space charge solver
- TEM3P – EM, thermal, and mechanical solver
- Gun3P – electrostatic field solver for DC guns

In this paper we will summarize various code integration efforts and new capabilities of the ACE3P code suite. We present an overview of recent efforts in code-integration of Geant4 with ACE3P for the study of dark currents [3] and a new python-based workflow based on the Lightsource Unified Modeling Environment (LUME) [4].

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ACE3P-GEANT4 INTEGRATION

The particle and radiation transport code Geant4 enables the calculation of radiation dosage collected externally to accelerator components. This code integration was recently used to provide valuable insight into dark current radiation studies for a 56-cell accelerator structure at KEK [3]. An overview of the code workflow setup (Fig. 1) and results of the full integrated study are shown (Fig. 2).

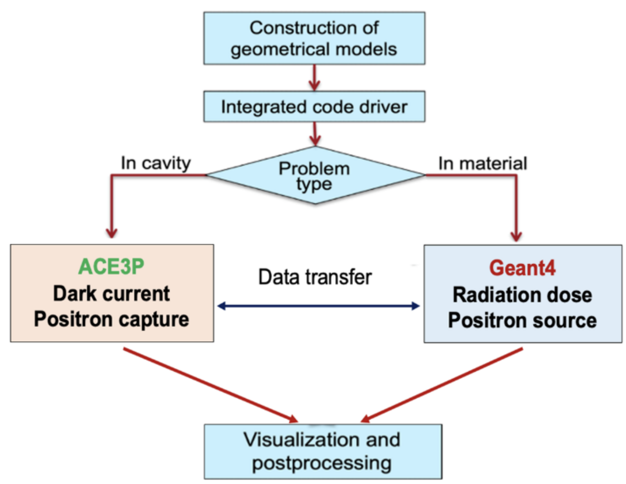

Figure 1: ACE3P-Geant4 code integration overview.

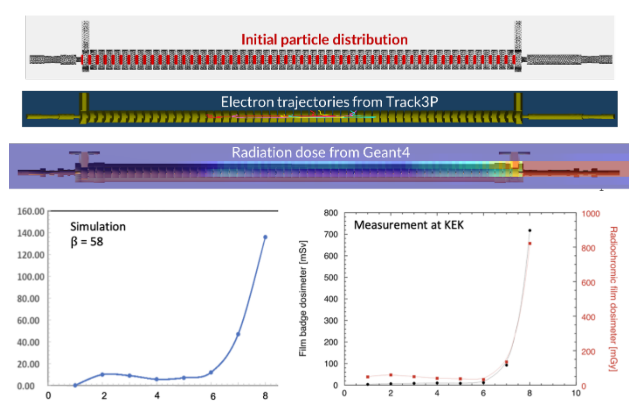

Figure 2: (Top) initial particle distribution, Track3P electron trajectories, and radiation pattern from Geant4. (Bottom) comparison of simulated radiation dose by monitor location and actual measurements taken from the monitors placed around the structure.

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LUME-ACE3P

The LUME project is built on a python code framework which enables input and output manipulation for various codes such as IMPACT and ASTRA [4]. By extending the base command wrapper classes defined therein, LUME-ACE3P [5] provides the necessary code interfaces for ACE3P and associated software such as Cubit and Acdtool, a helper utility for ACE3P. The primary use for LUME-ACE3P tools is to provide a simple and easy-to-use method for running parameter sweeps or optimization problems involving ACE3P codes.

General Workflow Setup

The primary workflow for LUME-ACE3P consists of generating a mesh from a geometrical model with Cubit, solving for fields on that mesh with an ACE3P module, and postprocessing the results for visualization or optimization. To set up the workflow, a user must provide a YAML-formatted configuration file, a Cubit-formatted journal file, an ACE3P module input file, and optionally an Acdtool postprocess input file.

The LUME-ACE3P configuration file contains all the information for the workflow such as file names, working directories, HPC options, etc. The configuration file is used as the input for the workflow using a python script with outputs collected in a formatted text file (Fig. 3).

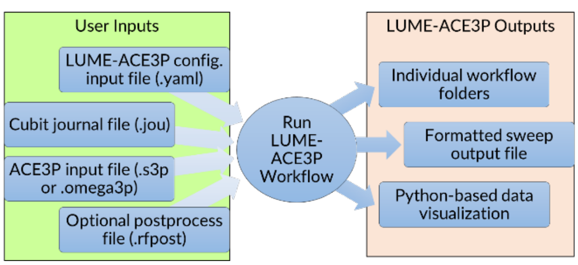

Figure 3: LUME-ACE3P input/output hierarchy.

Parameter Sweep Example

To set up a LUME-ACE3P to sweep a parameter, or set of parameters, an input dictionary is provided in the configuration file which specifies the range of values to sweep. The variable names must exactly match those found in the user-provided Cubit journal file but LUME-ACE3P will automatically update parameter values within the journal and generate new meshes for ACE3P. Contents for a typical parameter sweep is shown in Fig. 4.

The workflow parameters section contains HPC options (e.g. number of MPI tasks and cores ACE3P should use), directory preferences, and which ACE3P module to use. The input parameters section defines which variable names to be swept and parse the results to a specified output file.

This text output file will contain all the scattering matrix data from S3P at each of the parameter combinations. Additionally, a plotting utility is provided with LUME-ACE3P to view this data with interactive sliders to select from the input parameter ranges and between different scattering matrix entries (Fig 5).

```
workflow_parameters :
  'mode' : 'parameter_sweep'
  'module' : 's3p'
  'cubit_input' : 'bend-90degree.jou'
  'ace3p_input' : 'bend-90degree.s3p'
  'ace3p_tasks' : 32
  'ace3p_cores' : 4
  'ace3p_opts' : '--cpu-bind=cores'
  'workdir' : 'lume-ace3p_s3p_workdir'
  'workdir_mode' : 'auto'
  'sweep_output' : True
  'sweep_output_file' : 's3p_sweep_output.txt'
input_parameters :
  'cornercut' :
    'min' : 12.0
    'max' : 16.0
    'num' : 5
  'rcorner2' :
    'min' : 4.0
    'max' : 16.0
    'num' : 3
```

Figure 4: A sample LUME-ACE3P configuration file for parameter sweeping using S3P. The input parameters contain the names of the Cubit variables to sweep over.

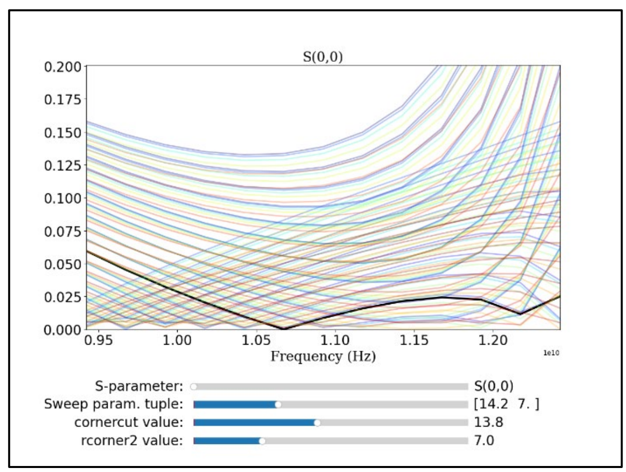

Figure 5: A sweep output plotting utility for S3P provided with LUME-ACE3P with interactive sliders.

Optimization Example

For optimization, LUME-ACE3P builds upon the Xopt code library [6] to provide various optimization generators for selecting new parameter query points from previous data. The configuration file is mostly the same as in the parameter sweeping case but instead of an input range, it provides a VOCs (Variables, Objectives, Constraints) object for Xopt to process, as well as other Xopt settings.

For a particular example, we examined toy model of a 90-degree bend in a rectangular waveguide with varying width “wgwidth” and corner chamfer length “cornercut”. The optimization objective was to minimize the S_{11} parameter at a specified frequency of 12 GHz [7].

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To test LUME-ACE3P with Xopt, we used a Nelder-Mead generator to select input data within the parameter space to locate the minimum S_{11} value. We also performed a fine parameter sweep of the two input variables to highlight the performance of the optimizer. (Fig. 6). Lastly, the individual S3P runs at specific inputs can be plotted versus frequency and iteration number with an interactive tool provided by LUME-ACE3P (Fig. 7).

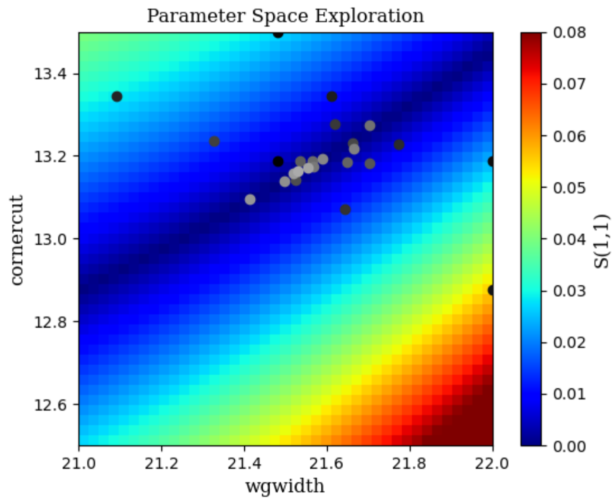

Figure 6: Parameter sweep of S_{11} at 12 GHz of a S3P toy model of a 90-degree bend. The optimizer steps are shown as grayscale dots increasing in brightness with iteration.

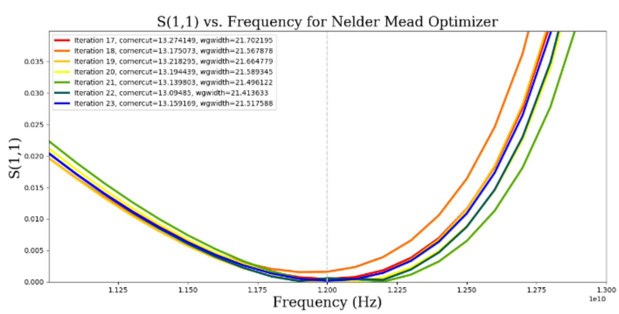

Figure 7: S-parameter plot vs frequency for the last few iterations of the optimization.

DISPERSIVE MATERIALS

A new modeling capability for ACE3P includes linear and non-linear dispersive materials for the study of new material types, is currently in development. Some preliminary results using a Lorentzian dispersive material in a rectangular waveguide have shown agreement between S3P and Ansys HFSS (Fig. 8).

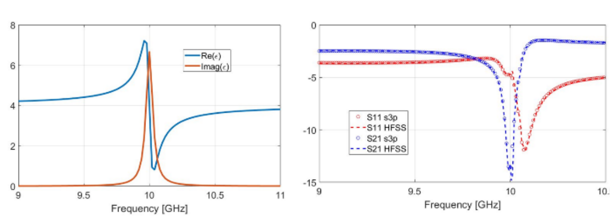

Figure 8: (Left) Lorentzian dispersion function. (Right) S_{11} and S_{21} S-parameters computed by S3P and Ansys HFSS.

DYNAMIC MODE DECOMPOSITION

Dynamic mode decomposition (DMD) is a new method for computing large-timescale dynamics from a subset of temporal data snapshots [8]. By computing electromagnetic field evolution after any transient effects, DMD can be used to reconstruct field solutions at arbitrary large times with great accuracy, depending on the number of modes and time snapshots.

By using DMD with snapshots generated from T3P, an alternate method for obtaining many cavity eigenmodes can be approximated in a shorter time than by directly running Omega3P for many different frequencies (Fig. 9).

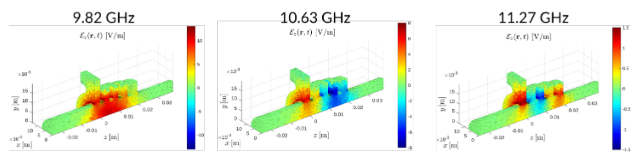

Figure 9: Several DMD modes computed from T3P time snapshots for a small cavity structure.

CONCLUSION

The ACE3P code suite continues to expand its capabilities for modeling new and complex physics as well as better integrate with existing software such as Geant4. Furthermore, new LUME-based workflow management tools provide increased user accessibility for using ACE3P on HPC systems such as NERSC's Perlmutter and SLAC's S3DF. These new tools provide the often-requested parameter-sweeping and optimization capabilities that are common in many commercial EM software packages.

Future work on LUME-ACE3P will enable parallel job submission, job error handling, checkpointing, plotting tools, and more. Also, code integration efforts will continue to add new software interfaces.

ACKNOWLEDGEMENTS

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