Taming the Ace3P RF simulation package for design work

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Comparing Omega3P with analytical results and HFSS 12.1.2 for a simple “pillbox” geometry

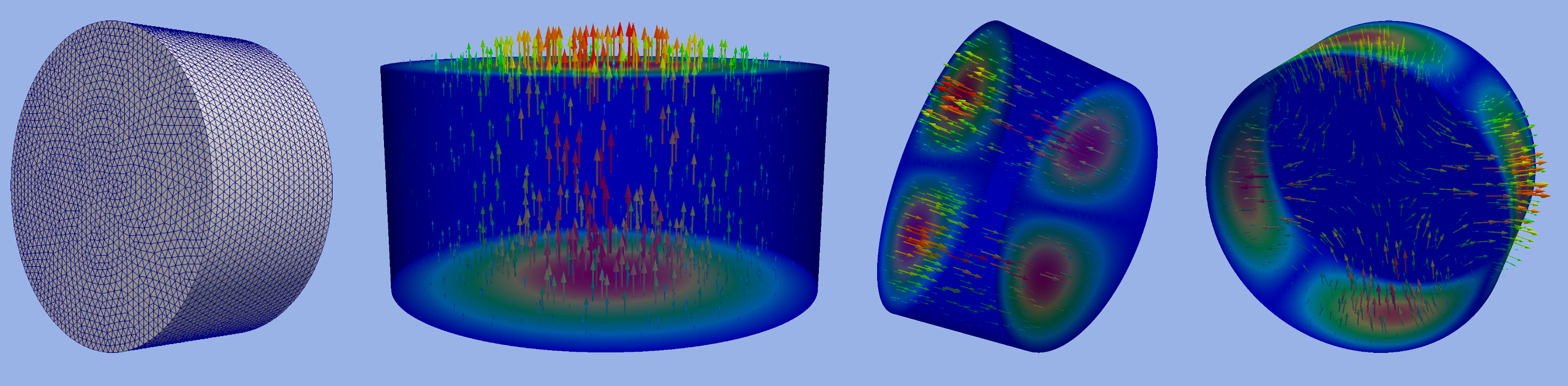
- As a first test, a cylindrical $R_c = 1\mathrm{m}, l = 1\mathrm{m}$ geometry was used
- The calculated frequencies and Q-factors for the different modes was compared with results from analytical formulas and HFSS 12.1.2
- TM_{mnp}-modes, analytical Q-factor:

$$Q_{mnp} = \frac{I_z \mu_0 \omega R_c \left[\left(\frac{m}{x_{mn}} \right)^2 \xi_1 I_{\theta s} + \xi_2 I_{\theta c} \right]}{R_s \left\{ 2R_c \left[\left(\frac{m}{x_{mn}} \right)^2 \xi_1 I_{\theta s} + \xi_2 I_{\theta c} \right] + {J'_m}^2 (x_{mn}) I_{\theta c} I_z \right\}}$$

- The analytical and numerical results match:

Mode name	f, O3P	f, HFSS	f, analytic	Q, O3P	Q, HFSS	Q, ana.
TM_{010}	1.14742	1.14746	1.14743	80996.62	81045.5	81045
TE_{111}	1.73742	1.73771	1.73742	92066.81	92221.4	-
TE_{111}	1.73742	1.73774	1.73742	92066.75	92219.5	-
TM_{110}	1.82824	1.82846	1.82824	102130.48	102305.0	-
TM_{110}	1.82824	1.82856	1.82824	102132.01	102303.0	-
TM_{011}	1.88772	1.88816	1.88772	69156.93	69300.7	69301
TE_{211}	2.09059	2.09137	2.09059	96425.12	969595.1	-
TE_{211}	2.09059	2.09151	2.09059	96426.03	96598.7	-
$\mathrm{TM}_{111}{}^*$	2.36419	2.36538	2.36418	77599.65	146262.0	-
$\mathrm{TM}_{111}{}^*$	2.36419	2.36543	2.36418	77401.99	82168.9	-

Frequencies in units of 10^8 Hz. Modes marked with “*” is mixed with TE_{011}



The mesh used, and field patterns for TM_{010}, TM_{110}, and TE_{211}.
Surface color indicating magnetic field magnitude, arrows electric field

Comparing Omega3P and HFSS for a CLIC T24 and TD24 single-cell geometry

- Before using Omega3P [1] for RF design, want to make check that results are the same as from HFSS
- Simulating a single cell with periodic boundary conditions
- Comparing key parameters:
  - Frequency
  - Q-factor
  - R/Q
  - Group velocity
  - Peak electric field
  - Peak magnetic field
  - Peak modified Poynting-vector S_c

What is S_c?

The modified Poynting vector S_c is a real time-constant vector-field, which gives an indication of likely breakdown sites [2].
This vector field is given as

$$\mathrm{S}_c = \mathrm{abs}(\Re(\tilde{\mathrm{S}})) + \frac{1}{6}\mathrm{abs}(\Im(\tilde{\mathrm{S}}))$$

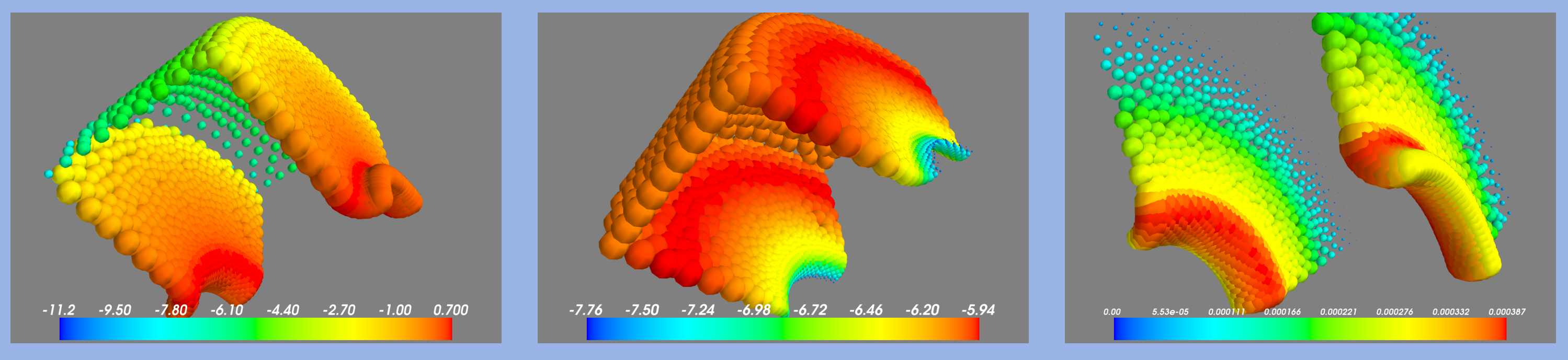
where the absolute value is taken componentwise, and $\tilde{S}$ is the complex Poynting vector

$$\tilde{\mathrm{S}} = \frac{1}{2}\mathrm{E} \times \mathrm{H}^*$$

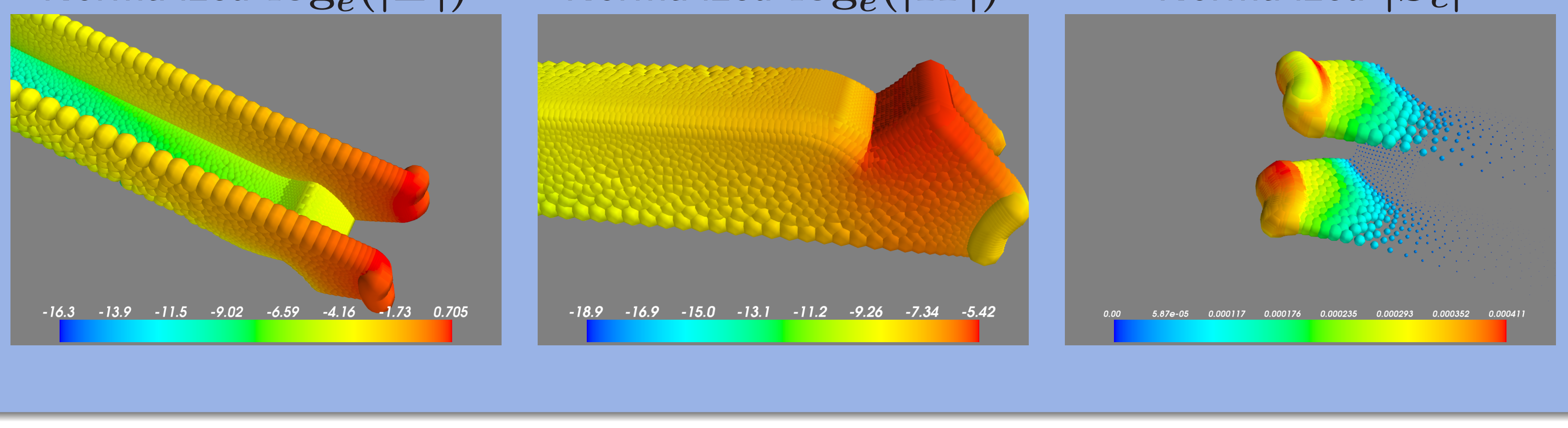
Calculation	Frequency	Q-factor	R/Q	v_g	$\lvert\mathrm{E}\rvert_{\max}$	$\lvert\mathrm{H}\rvert_{\max}$	$\lvert\mathrm{S}_c\rvert_{\max}$
T24/M1, P=2	11.99470	6652.48	15978.42	1.7570	2.09390	2.82237	0.401831
T24/M2, P=1	11.98682	6645.12	15947.36	1.7751	2.23270	3.42246	0.599280
T24/M2, P=2	11.99477	6653.70	15978.30	1.8165	2.08956	2.64085	0.395954
T24/3, P=2	11.99477	6653.84	15978.30	1.8170	2.05856	2.64120	0.396020
T24/4, P=2	11.99477	6655.21	15978.18	1.8178	2.04253	2.63874	0.395114
T24/HFSS	11.995	6600.	15956.	1.83	1.95	2.6	0.37
TD24/M1,P=2	11.99472	5532.	14560.79	1.652	2.17452	5.29	0.421
TD24/M2,P=2	11.99484	5541.	14559.71	1.654	2.07334	1.654	0.417
TD24/HFSS	11.9942	5536.	14587.	1.65	1.95	4.1	0.41

- Peak E dimensionless, peak H and S_c in units of mA/V. Frequency in GHz, R/Q in Ω/m (linac def.), v_g in % of c. Edge lengths in $\mu\mathrm{m}$.
- All peak fields normalised using mean accelerating gradient $\langle E_z \rangle$

Mesh	# Elem.	Iris roundoff edge length	DWG neck edge length
T24/M1	41321	400	-
T24/M2	46088	200	-
T24/M3	47646	200	-
T24/M4	73473	100	-
TD24/M1	24364	300	600
TD24/M2	61655	150	300



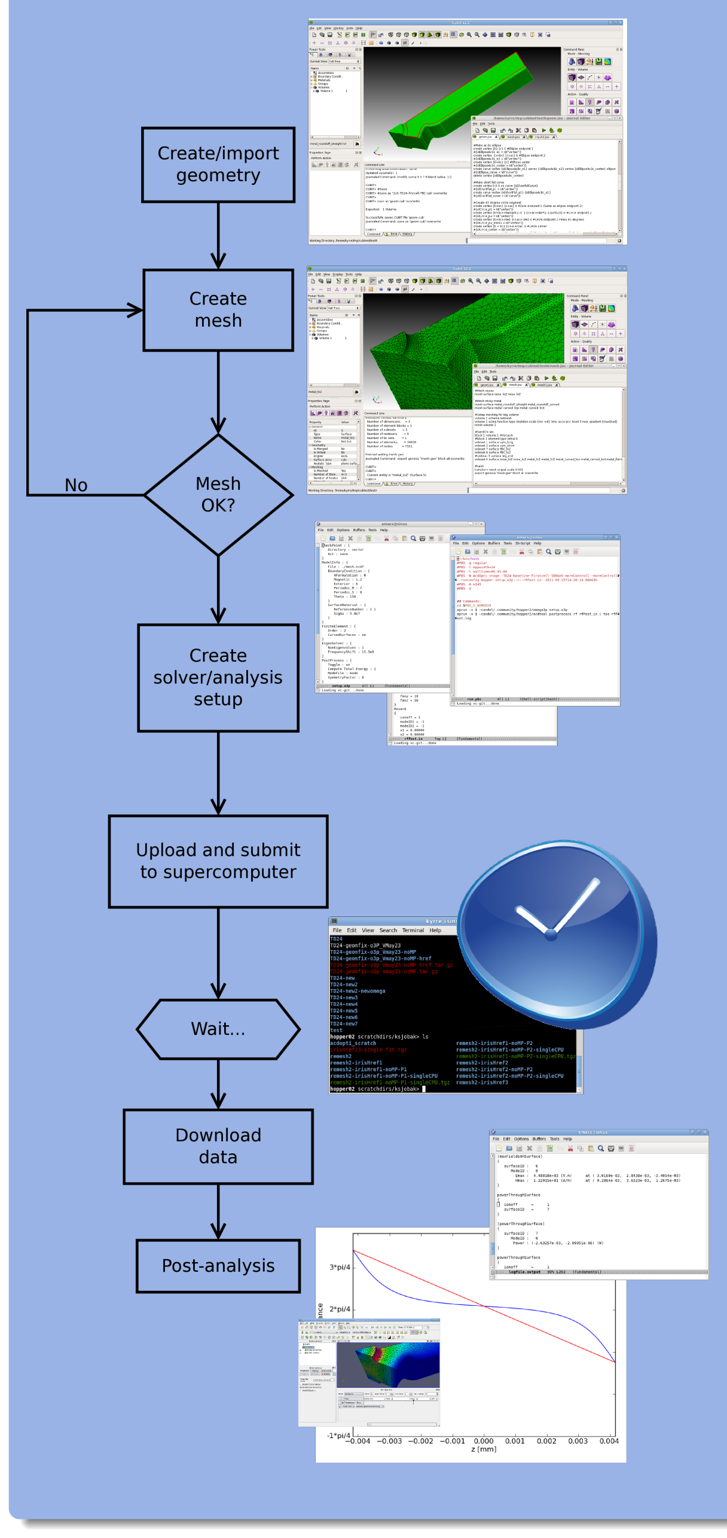
Normalized $\log_e(\lvert E\rvert)$ Normalized $\log_e(\lvert H\rvert)$ Normalized $\lvert S_c\rvert$



What is ACE3P?

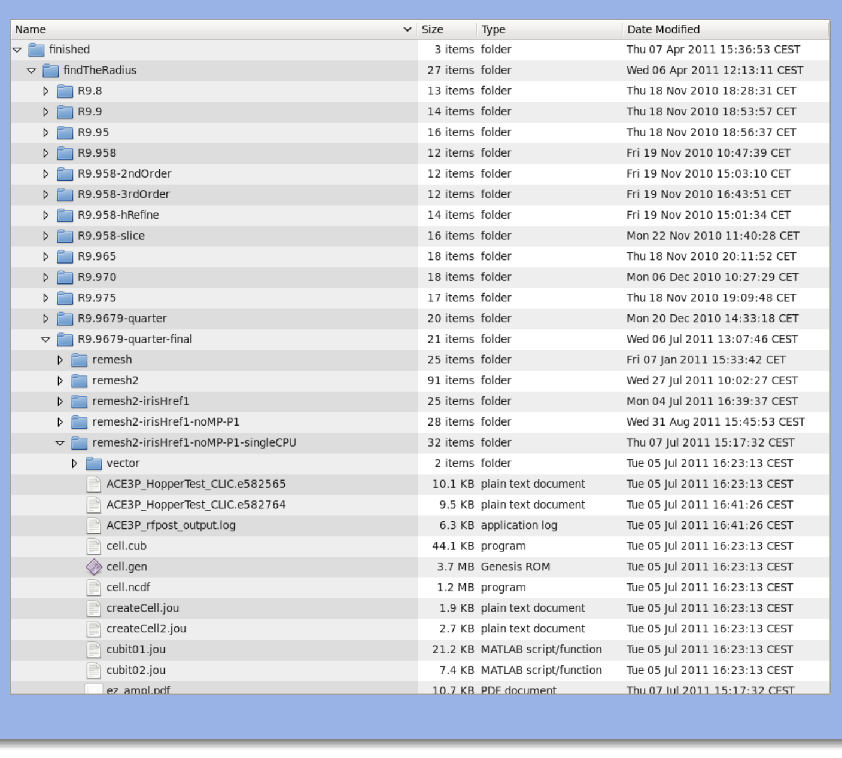
- Ace3P (Advanced Computational Electromagnetics 3P) is a suite of finite element solvers capable of calculating several parameters relevant to RF design and diagnostics:
  - Cavity eigenmodes (Omega3P)
  - Transient response to beam (Tau3P)
  - Particle tracking with surface physics (Track3P)
  - S-parameters (S3P)
  - Particle-in-cell simulation of beam (Pic3P)
  - Multi-physics for integral EM and thermal/mechanical analysis (Temp3P)
- Scalable to thousands of CPU cores, enables handling of large-scale problems
- Uses conformal higher-order tetrahedral elements
- Developed by the Advanced Computations Group (ACD) at SLAC [3]

The challenge with Ace3P: It’s user-interface



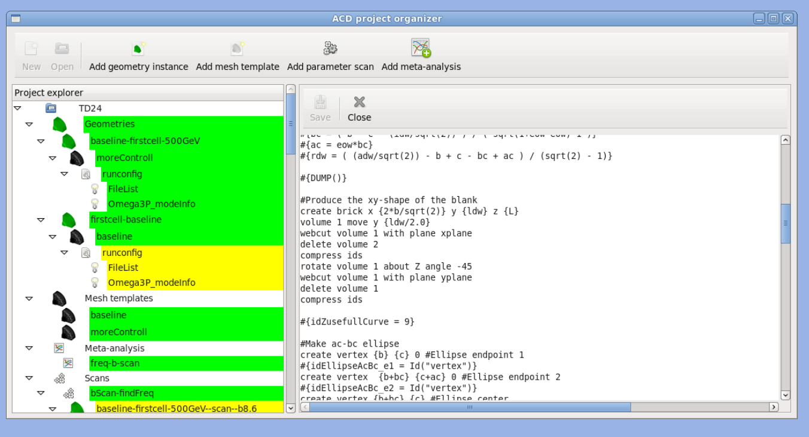
- Setting up an ACE3P simulation requires many steps
- Many of them manual and error-prone
- Running many simulations produces a lot of files; easy to loose track of differences
- No simple way to compare results between simulations

Difficult to use for work requiring fast turn-around, such as design and optimisation of RF components

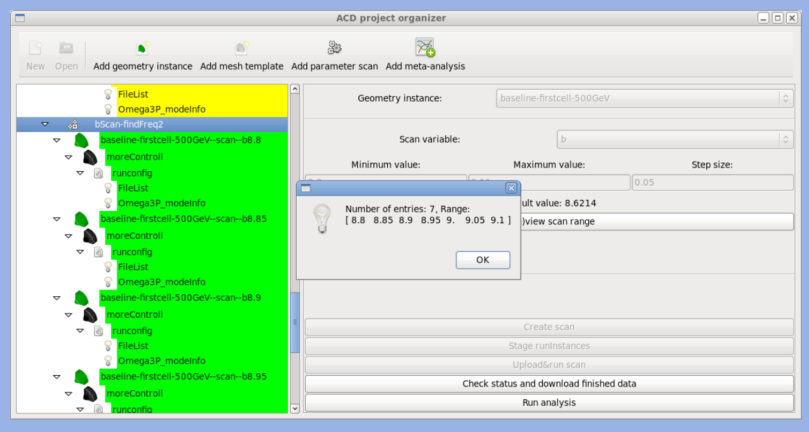


Making life easier: AcdOpti

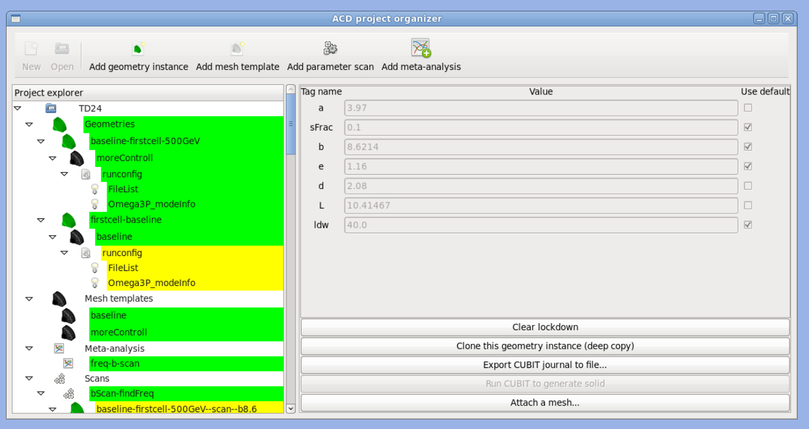
- Automates the steps for setting up and running an ACE3P simulation
- Organises the in- and output data
- This enables fast turnaround of simulations, enabling design of RF components
- First goal is to design a tapered damped accelerating structure for a 500 GeV CLIC



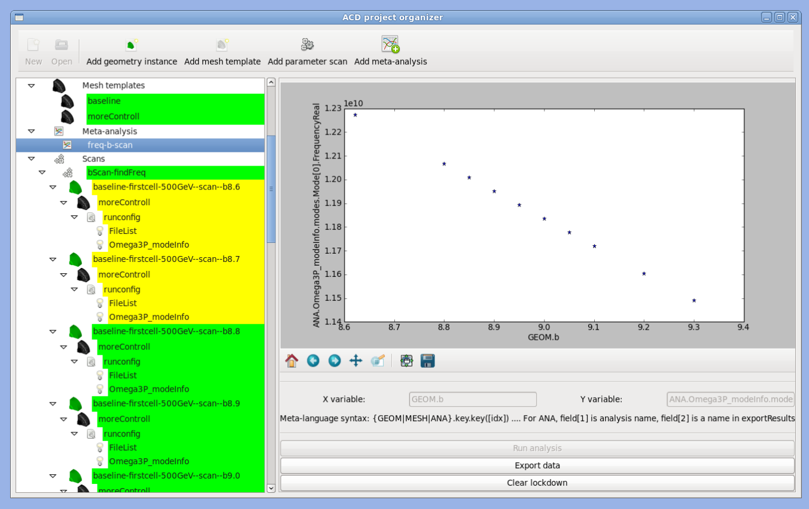
Setup CUBIT scripts



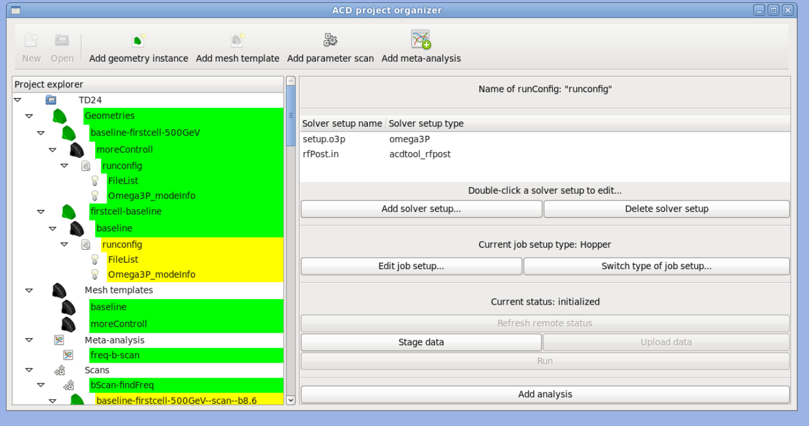
Scan a geometry parameter



Set parameters for geometry and mesh



Plot geometry parameters, mesh parameters, and analysis results against each other over multiple simulations



Create solver setup and submit, run, and fetch job at remote cluster

`https://github.com/kyrsjo/AcdOpti`

References

[1] Cho Ng Lie-Quan Lee, Zenghai Li and Kwok Ko. Omega3p: A parallel finite-element eigenmode analysis code for accelerator cavities. *SLAC-PUB 13529*, 2009

[2] A. Grudiev, S. Calatroni, and W. Wuench. New local field quantity describing the high gradient limit of accelerating structures. *Phys. Rev. ST Accel. Beams*, October 2009

[3] `https://slacportal.slac.stanford.edu/sites/ard_public/acd/Pages/Default.aspx`

CERN accelerator school 2011, Chios

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