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TIME-DEPENDENT, THREE-DIMENSIONAL SIMULATION OF FREE-ELECTRON LASER OSCILLATORS*

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CODE CHARACTERISTICS

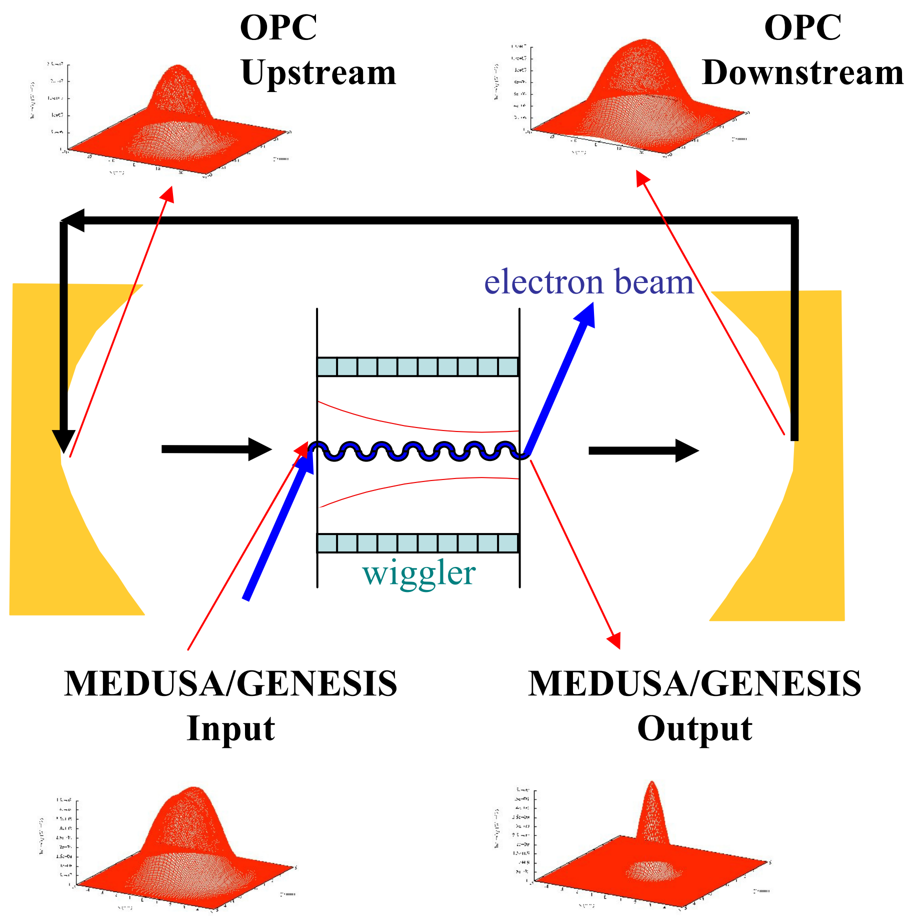
OPC: Fortran 90/PERL User Interface (http://lpno.tnw.utwente.nl/opc.html)

- Optical Propagation by either Spectral Method or Fresnel Diffraction Integrals
- Parallelized
- Gain Models (MEDUSA, GENESIS)
- Diagnostics: field profile, cross section, Power/Energy vs time & position
- Optical Elements: mirrors, lenses, phase masks, diaphragms
- Out-Coupling: edge, transmissive, hole
- Distortion/Misalignments
- Single Slice/Time Dependence

MEDUSA (Fortran 90)	**GENESIS** (Fortran 77)
Slowly-Varying Envelope Approximation	Slowly-Varying Envelope Approximation
Gaussian Modal Expansion	Field Solver on Cartesian Grid
Non-Wiggler-Averaged Orbits	Wiggler-Averaged Orbits
Single Slice/Time Dependence	Single Slice/Time Dependence
Start-Up From Noise	Start-Up From Noise
Harmonics	Harmonics
Parallelized	Parallelized

NUMERICAL PROCEDURE

- Interfaces written between MEDUSA/OPC & GENESIS/OPC.
- MEDUSA/GENESIS simulate the interaction in the wiggler and write the complex phase front at the wiggler exit to a file that is handed off to OPC.
- OPC propagates the field around the resonator and hands off the complex phase front at the wiggler entrance to MEDUSA/GENESIS.



- MEDUSA writes the phase front at the output of the wiggler directly into the input file for OPC, but uses a translator to decompose the complex phase front at the wiggler entrance from OPC back into Gaussian optical modes and then write a new input file.
- GENESIS uses the same grid (size and number of mesh points) as used in OPC so no translators are necessary.

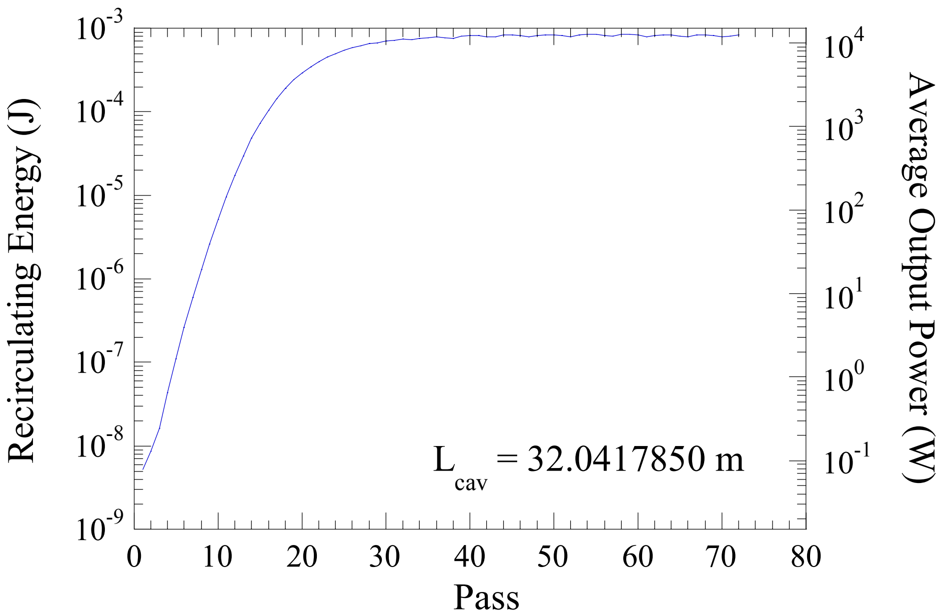
JEFFERSON LAB EXPERIMENT

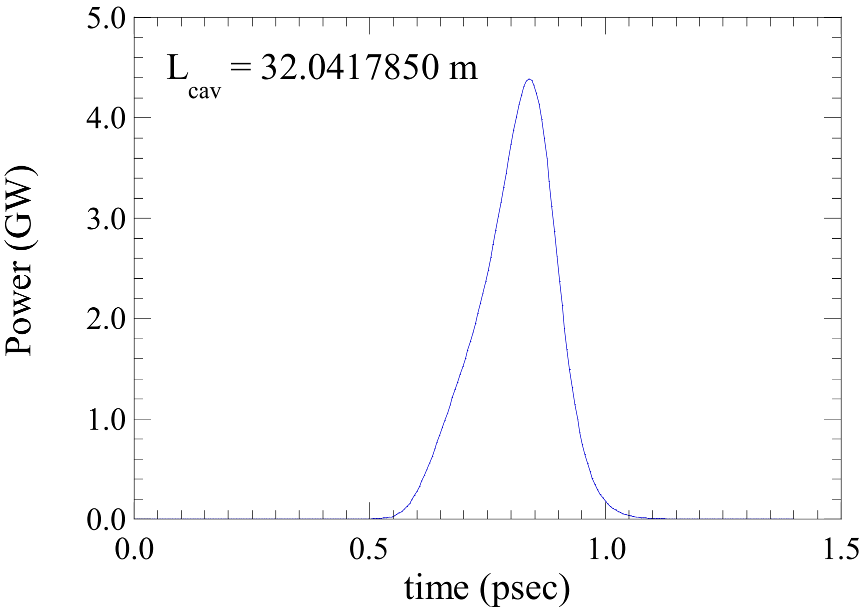
- We validate MEDUSA/OPC using the parameters of the 10-kW Upgrade Experiment at Jefferson Lab [G. Neil *et al*., Nucl. Instrum. Methods Phys. Res. **A557**, 9 (2006)] for time-dependent (*i.e*., 4-D) simulations.
- The nominal parameters are:

Electron Beam	
Beam Energy:	115 MeV
Bunch Charge:	115 pC
Bunch Length:	390 fsec
Bunch Frequency:	74.85 MHz
Emittance:	9 mm-mrad (wiggle plane), 7 mm-mrad
Energy Spread:	0.3%
Wiggler	
Period:	5.5 cm
Amplitude:	3.75 kG
Length:	30 periods
Radiation/Resonator	
Wavelength:	1.6 microns
Resonator Length:	32 m
Rayleigh Range:	0.75 m
Out-Coupling:	21% (transmissive)

PULSE GROWTH & TEMPORAL SHAPE

Typical simulations show a region of exponential growth that rolls over to reach a long-term steady state. Oscillations in the pulse energy/power are seen, and corresponds to an oscillation in the position of the mode waist (more later).





The pulse shapes are found to be smooth and distorted from a symmetric pulse due to slippage and the cavity tuning.

CAVITY TUNING & PERFORMANCE

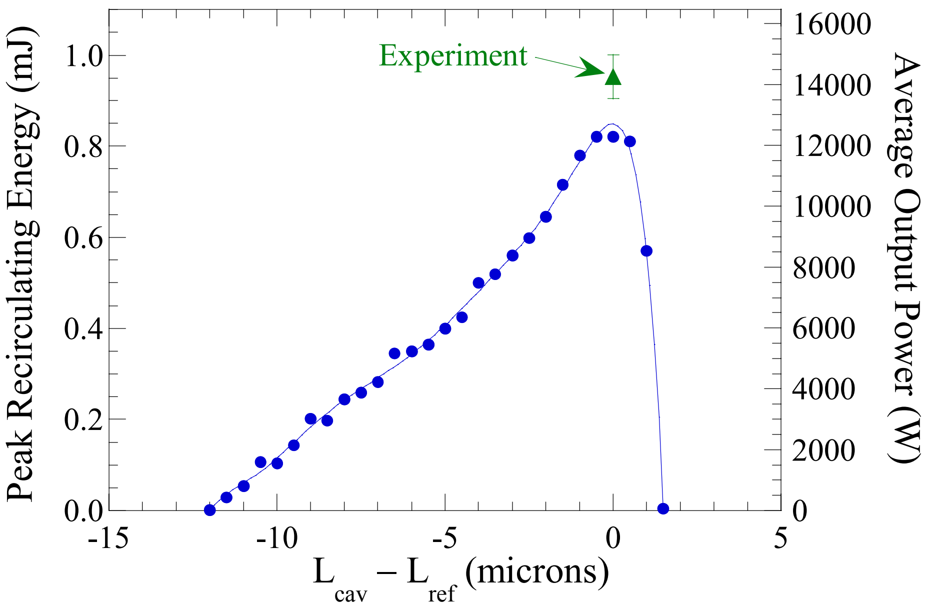
• Comparison of the cavity tuning curve with the observed optimal cavity tuning and power show good agreement. **The experiment records 14.3 ± 0.72 kW, and the simulation finds 12.3 kW** at the optimal cavity length.

• No complete cavity tuning curve is available from the experiment, but there is agreement as to the width of the tuning curve and the shape.

- **The width seen in simulation and the experiment is about 12-13 microns.**
- **The shape of the tuning curve is not sharply peaked but, rather, is triangular in both the experiment and the simulation.**

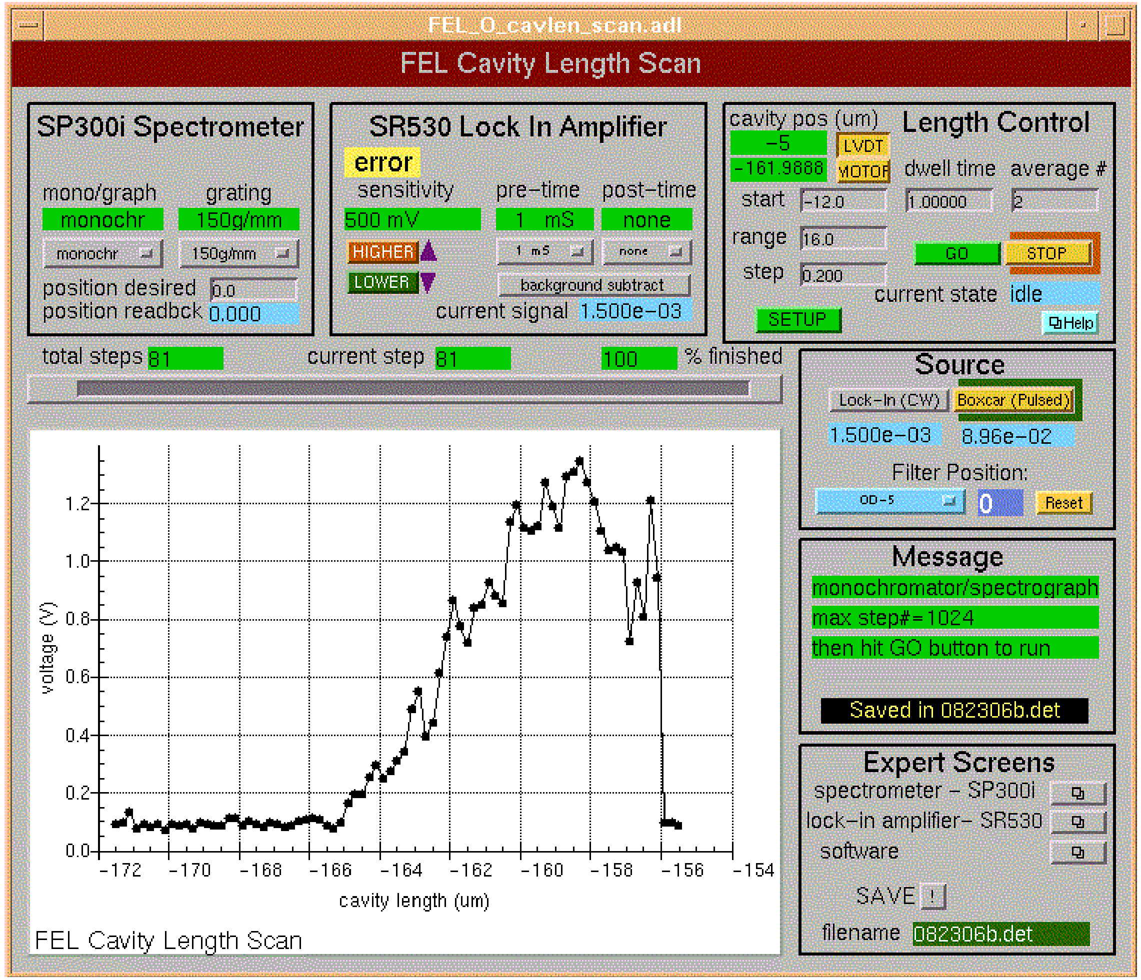
• The exact optimal cavity length in the experiment is not known. In addition, the zero-detuning condition ($L_{cav} = \upsilon_{gr}/2f_{rep}$) is not a precise calculation because the group velocity in the wiggler is not known.

- Because of this, we use L_{ref} to correspond to the optimal cavity length found in simulation.



PULSED MODE CAVITY SCAN

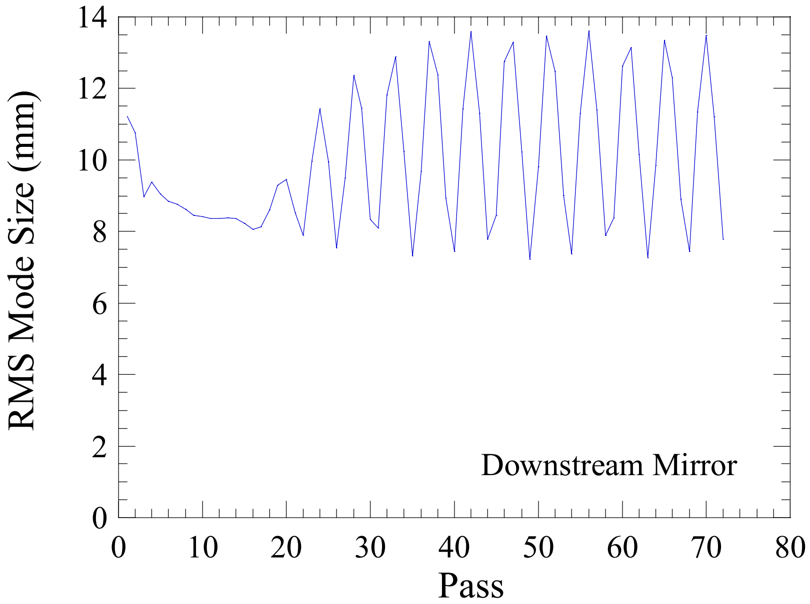
- Absorption on the mirrors and mirror mounts in the CW mode causes mirror steering problems
  - Makes it difficult to perform accurate cavity tuning scan in CW mode
  - Cavity tuning scan done in pulsed mode – not directly comparable

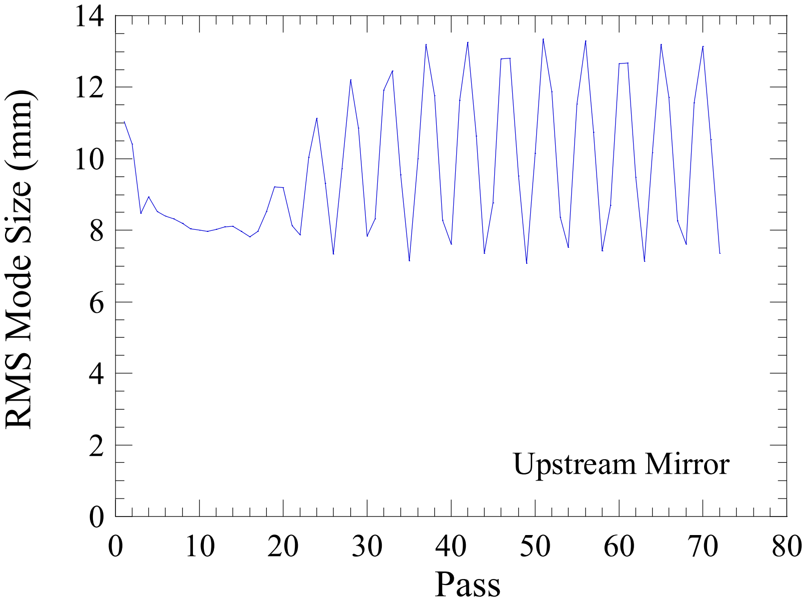


- Raw data from pulsed mode cavity length scan shown at right
  - 10% output coupler
- Data shows roughly “triangular” shape for the tuning curve
- Data shows a full width cavity tuning range of about 10 µm.

OPTICAL MODE SIZE

The optical mode size on the up- and down-stream mirrors oscillates about an average of about 10 - 11 mm. **This average is in accord with observations**. No diagnostic to observe the oscillations currently exists. The oscillations correspond to similar oscillations in the gain and pulse energy, where the minimum (maximum) in the spot size corresponds to a maximum (minimum) in the pulse energy.



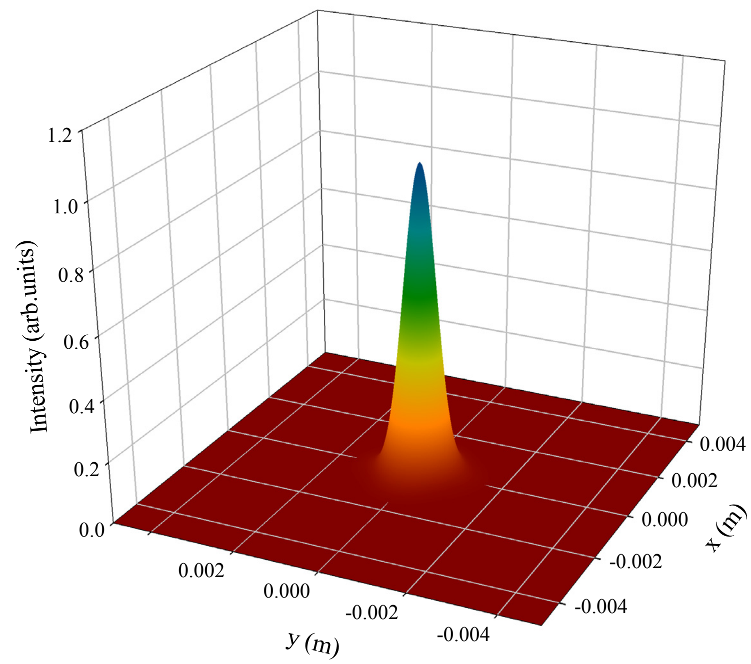


The oscillation appears to be due to an oscillation in the location of the mode waist. Optical guiding results in a mode size at the wiggler exit which may be either larger or smaller than the empty resonator mode, and this affects the location of the waist, which no longer coincides with the center of the resonator. In other words, the mode is no longer symmetric within the resonator.

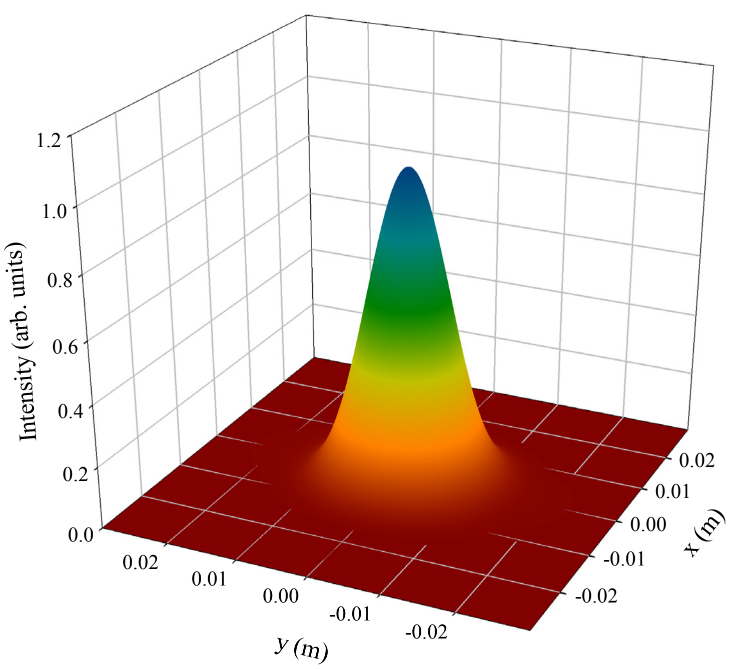
OPTICAL MODE SHAPE

The mode purity at the wiggler exit looks good, and the mode appears to have a near-Gaussian shape, that expands as it propagates to the downstream mirror

Wiggler Exit



Downstream Mirror



There is no M^2 diagnostic at present in MEDUSA/OPC or in the experiment, but we conclude that the M^2 for this case must be near unity.

JAERI EXPERIMENT

- We chose to use the JAERI FEL [N. Nishimori, Proc. FEL 2006, Berlin, Germany, Paper TUAAU03] to benchmark MEDUSA/OPC and GENESIS/OPC.
  - For benchmark purposes, we make some simplifications of the parameters, so the results are only nominally those of the experiment
- The basic parameters we use are as follows:

Electron Beam

Beam Energy:	16.8 MeV
Bunch Charge:	0.4 nC
Peak Current:	35 A
Bunch Length:	17.34 psec
Bunch Frequency:	20.825 MHz
Emittance:	40 mm-mrad
Energy Spread:	1.5%

Wiggler

Period:	3.3 cm
Amplitude:	3.213 kG
K_{rms}:	0.7
Length:	52 periods
Type:	Weak focusing (2-plane)

Radiation/Resonator

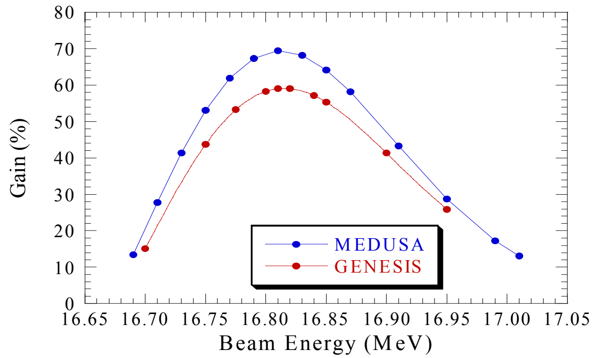
Wavelength:	22 microns
Resonator Length:	7.2 m
Rayleigh Range:	1.0 m
Out-Coupling/Losses:	3%

- Simplifications
  - Zero energy spread in time-dependent simulations.
  - Transmissive out-coupling.
  - Two-plane focusing with beam matched to wiggler.

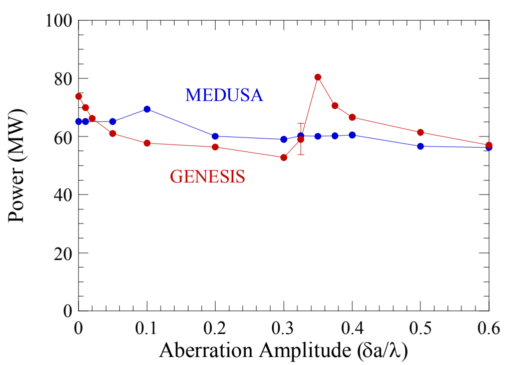
STEADY-STATE SIMULATIONS

Steady-state simulations are done with one time slice – so there is no slippage and there is no cavity-detuning. Reported at the 30th International FEL Conference.

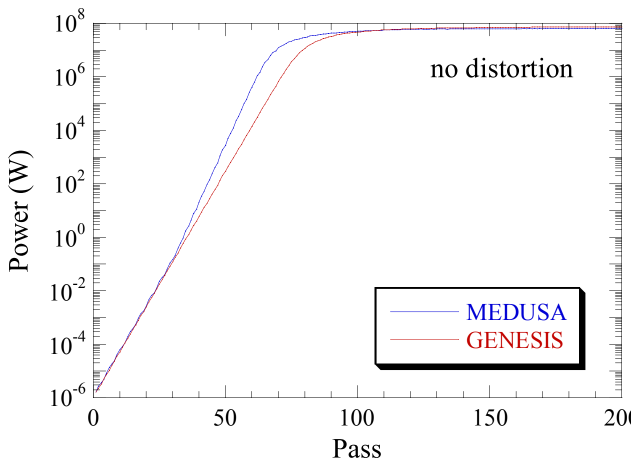
MEDUSA & GENESIS show good agreement for the single-pass gain



When fixed distortion is applied to both mirrors, MEDUSA/OPC & GENESIS/OPC show some discrepancies, but similar trends

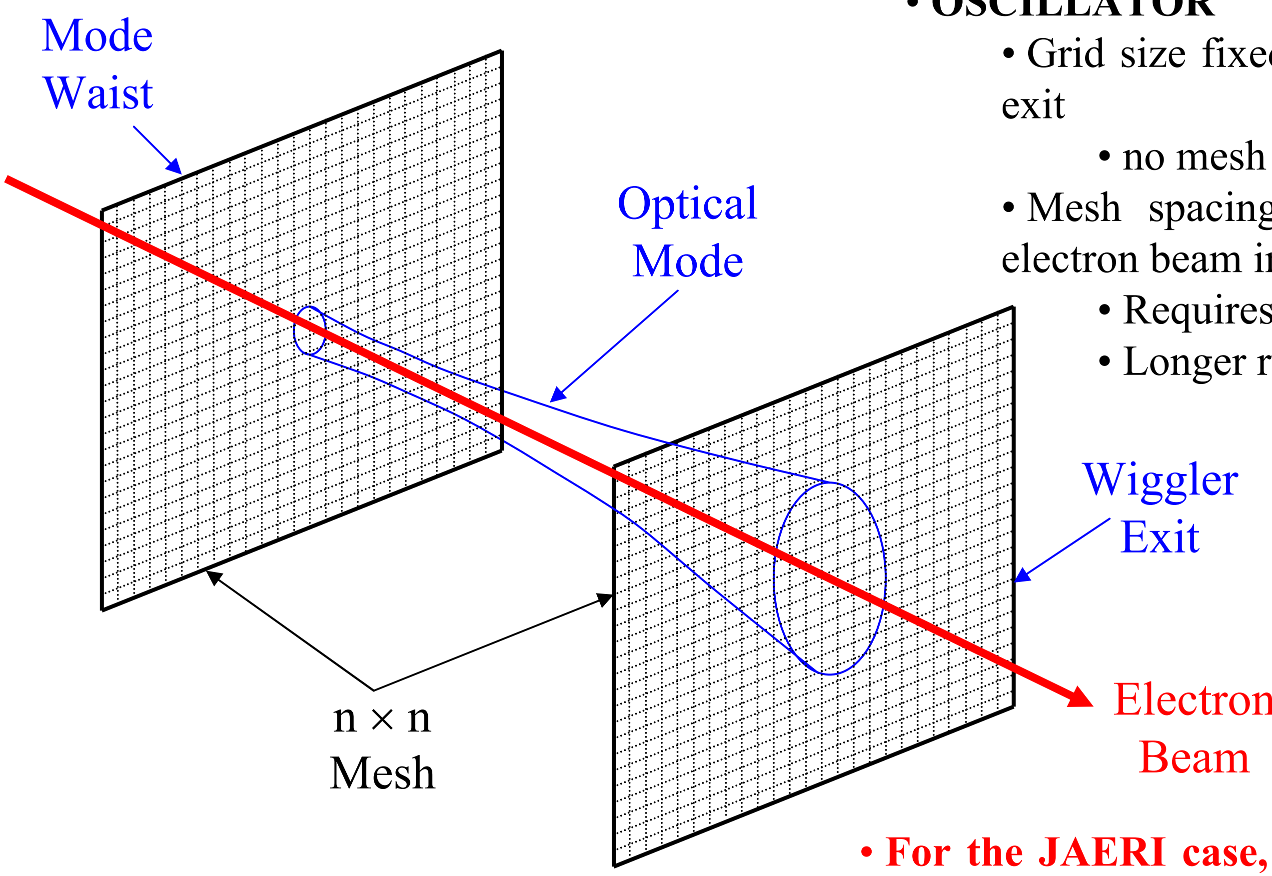


MEDUSA/OPC & GENESIS/OPC show good agreement for the growth to saturation and equilibrium power in the oscillator without distortion



Overall agreement between MEDUSA/OPC & GENESIS/OPC is encouraging for steady-state oscillator simulations

MESH: OSCILLATOR vs AMPLIFIER



- **OSCILLATOR**
  - Grid size fixed by optical mode at wiggler exit
    - no mesh refinement in wiggler
  - Mesh spacing fixed by need to resolve electron beam interaction
    - Requires very fine mesh
    - Longer run times

- **For the JAERI case, GENESIS/OPC needed a grid of 1024 × 1024**
  - **Run time scales as n^2**
  - **Worse for shorter Rayleigh ranges**
- **MEDUSA/OPC needed 15 modes for JAERI and 6 modes for JLab**
  - **run time scales linearly with number of modes**

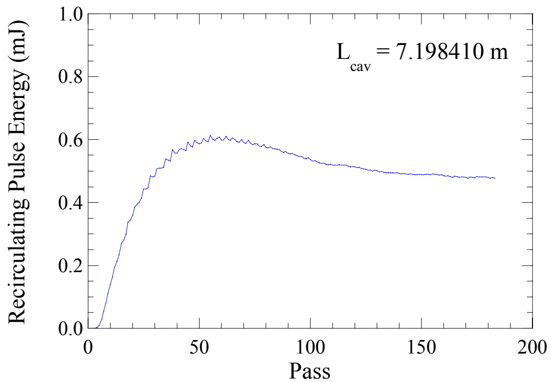
- **AMPLIFIER**
  - Optical mode guided inside wiggler
  - Need smaller mesh with fewer mesh points than in an oscillator
    - Faster run times

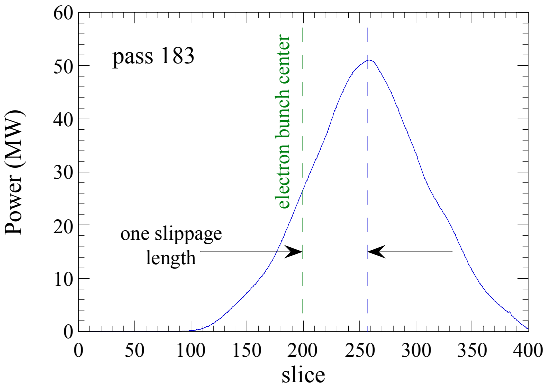
TIME-DEPENDENT SIMULATIONS

MEDUSA/OPC & GENESIS/OPC were run with bunch lengths of 17.34 psec, time windows of 29.35 psec and 400 slices. This means that the slices are "contiguous" in that the head-to-head separation between the slices is one wavelength. **Shot noise was not included and the runs were made with a small seed pulse**.

MEDUSA/OPC

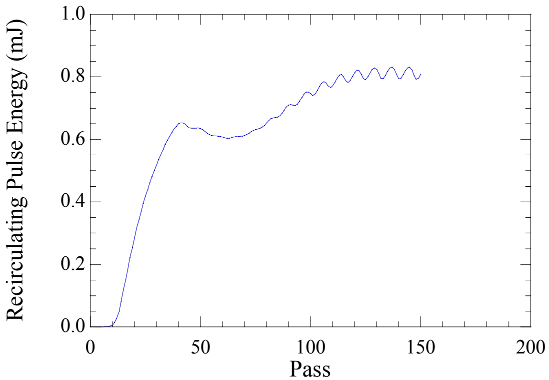
The pulse energy rises exponentially but rolls over and reaches an equilibrium after about 100 passes.





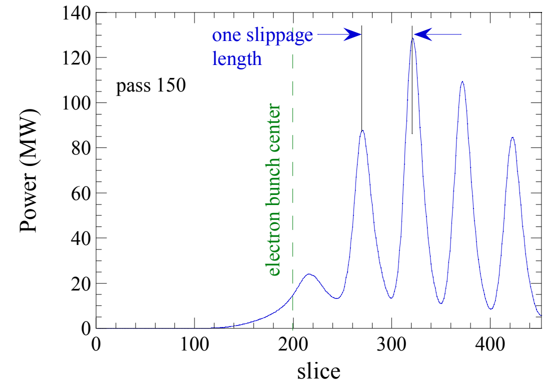
The pulse shape at equilibrium is smooth with a somewhat sharper leading edge, and at this cavity length leads the electron bunch by one slippage length.

GENESIS/OPC



Up to about pass 25, GENESIS & MEDUSA are on track. After that, the two codes increasingly diverge.

The discrepancy arises from the formation of intense regular spikes in the pulse, which also walks off the electron beam and out of the time window. **This is unphysical**.



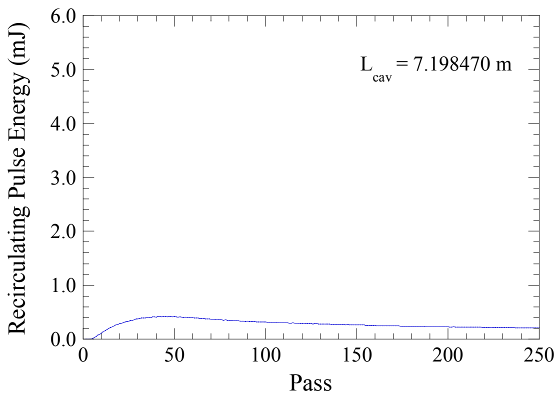
The cavity length for these runs corresponds to a cavity that was about 60 μm shorter than the zero detuning length.

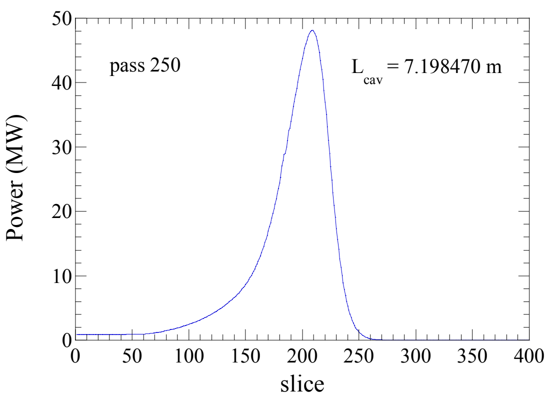
SIMULATION AT ZERO DETUNING

The discrepancy between MEDUSA/OPC and GENESIS/OPC grows wider at zero cavity detuning [$L_{cav} = c/2f_{rep}$].

MEDUSA/OPC

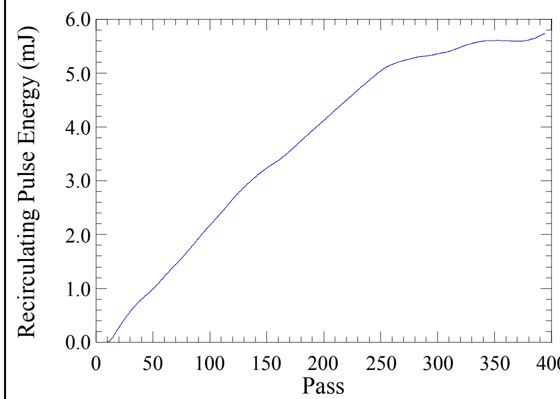
MEDUSA/OPC shows the power come to an equilibrium state, but this is on the downside of the tuning curve where the power is below the maximum.





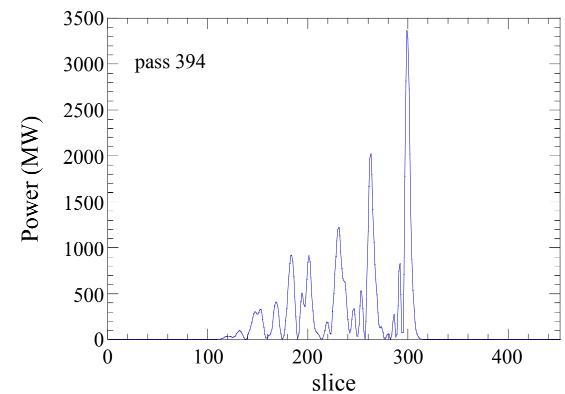
The pulse shape is regular with the expected distortion and exhibits a peak near the center of the electron bunch.

GENESIS/OPC



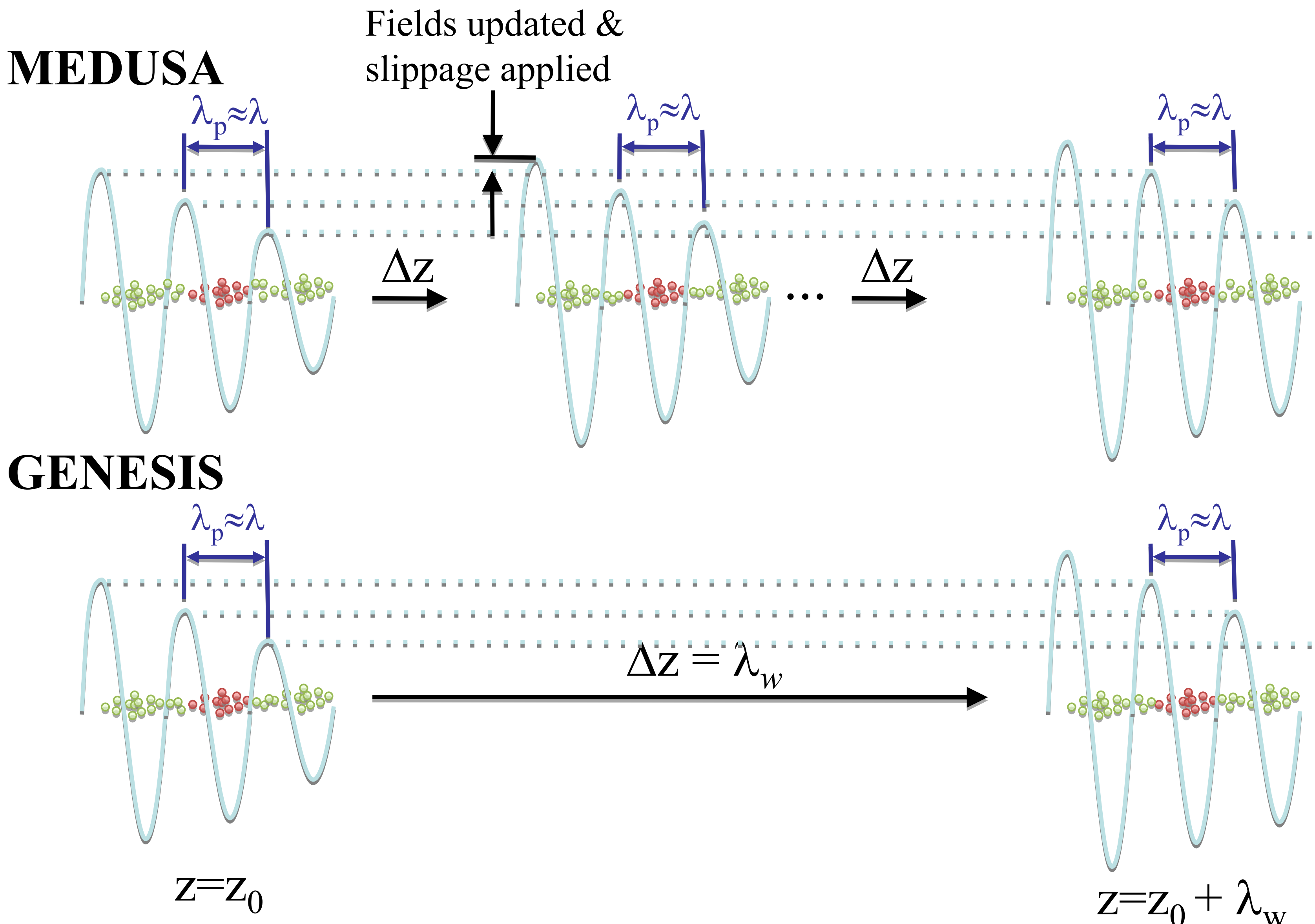
GENESIS/OPC shows the power increase slowly with no equilibrium state forming. The growth is just slightly above the loss rate, and reaches levels an order of magnitude greater than MEDUSA/OPC.

The pulse breaks up into intense spikes as before, but is now appears more chaotic and does not have regularly spaced spikes.



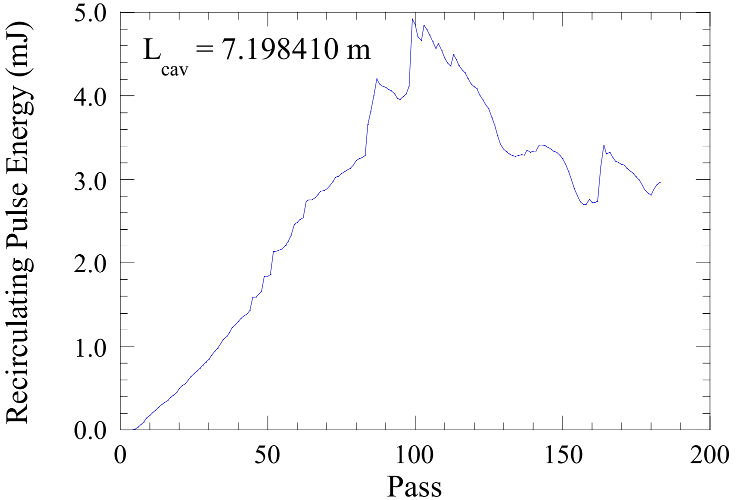
The GENESIS/OPC results are a numerical artifact. The source was not due to (1) too few particles, (2) too coarse a mesh, (3) pulse shape (Gaussian vs parabolic), (4) the number of slices, or (5) the integration step size. **It was found to be due to the way slippage is applied**.

SLIPPAGE COMPARISON

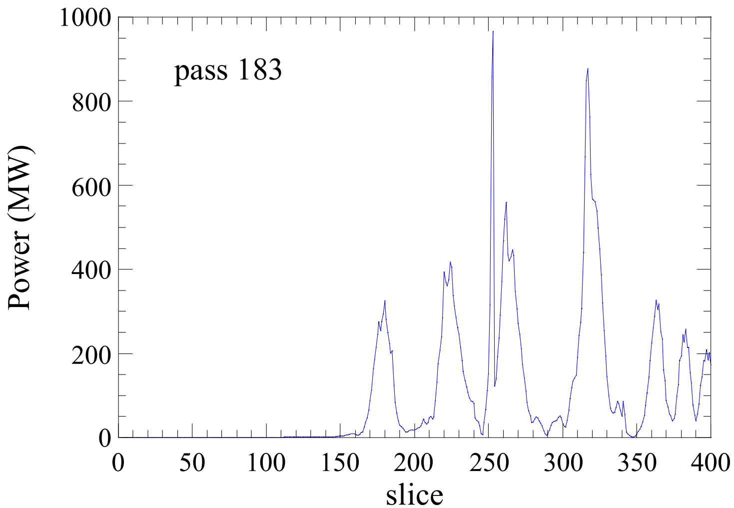


SLIPPAGE EVERY WIGGLER PERIOD

MEDUSA can be run with slippage applied at arbitrary intervals, but is typically run with fractional slippage applied on every integration step. The first test was to run MEDUSA/OPC with slippage applied once every wiggler period.



<u>Applying slippage once per wiggler period</u> results in an order of magnitude increase in the peak power as in GENESIS/OPC, and no clear equilibrium state.



The pulse shape also shows spikiness, and the leading edge of the pulse has slipped out of the electron beam and out of the time window.

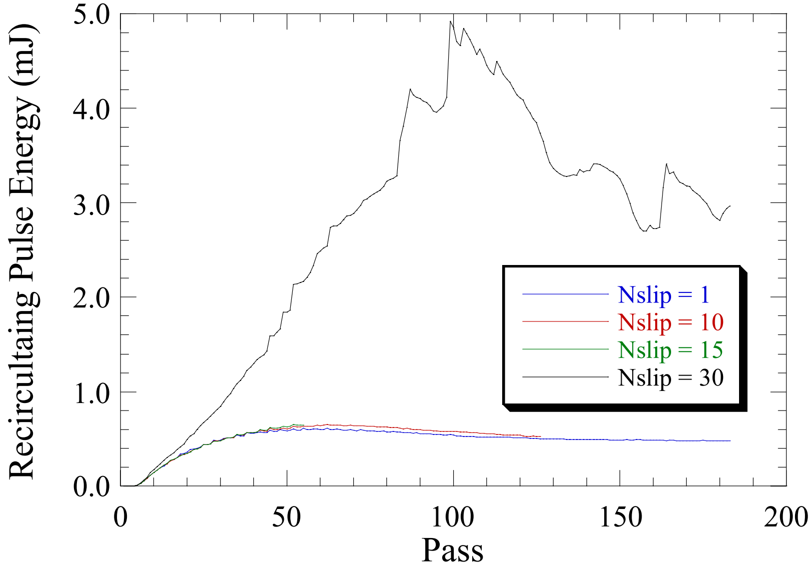
It is apparent that the source of the dramatically higher powers and seemingly chaotic spikes in GENESIS/OPC is the coarseness of the application of slippage. The next question is **"how frequent an application of slippage is required for numerical convergence?"**

SLIPPAGE CONVERGENCE TEST

We ran MEDUSA/OPC with applications of slippage at varying intervals of once per wiggler period and shorter for the JAERI and Jefferson Laboratory parameters..

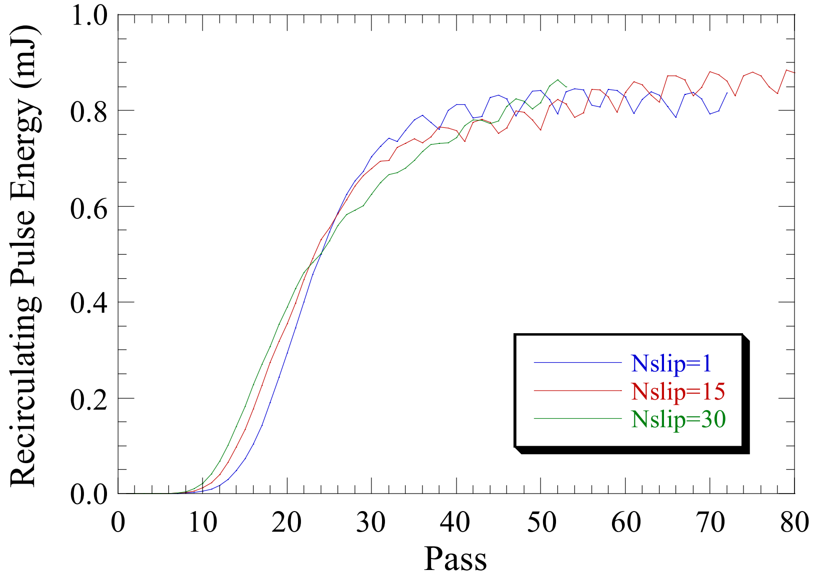
JAERI Parameters

Runs of MEDUSA/OPC for slippage applications more frequently than once per wiggler period show no spikiness and are in good agreement. Slightly higher powers are found as the interval between slippage applications increases.



Jefferson Lab Parameters

Runs of MEDUSA/OPC for the Jefferson Laboratory parameters do not exhibit spikiness and are in rough agreement as to the power, although the power climbs slightly with longer intervals between slippage.



What aspect of the parameters for the JAERI parameters give rise to the spikiness and dramatically higher power?

SLIPPAGE COMPARISON - SASE

- MEDUSA & PERSEO were used to compare shot noise algorithms for the fundamental & harmonics.
  - PERSEO uses KMR orbit analysis & applies slippage once per wiggler period.
  - PERSEO used 3-D phenomenological fit parameters to scale diffraction, filling-factor, and emittance.
  - Parameters consistent with SDL/BNL FEL using the NISUS wiggler.

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The effect of shot noise on the start up of the fundamental and harmonics in free-electron lasers

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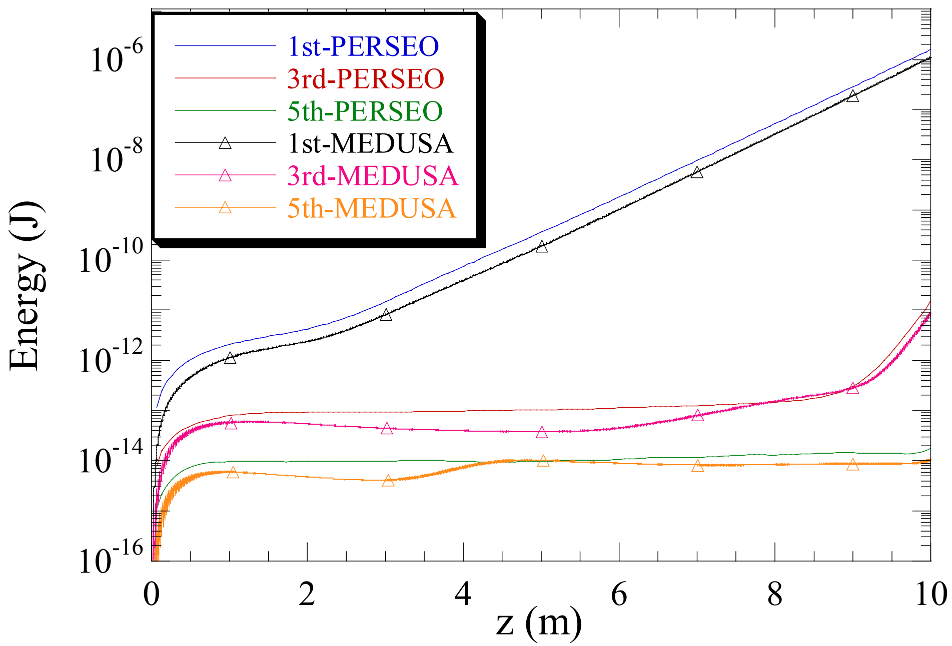
The problem of radiation start up in free-electron lasers (FELs) is important in the simulation of virtually all FEL configurations including oscillators and amplifiers in both seeded master oscillator power amplifier (MOPA) and self-amplified spontaneous emission (SASE) modes. Both oscillators and SASE FELs start up from spontaneous emission due to shot noise on the electron beam, which arises from the random fluctuations in the phase distribution of the electrons. The injected power in a MOPA is usually large enough to overwhelm the shot noise. However, this noise must be treated correctly in order to model the initial start up of the harmonics. In this paper, we discuss and compare two different shot noise models that are implemented in both one-dimensional wiggler-averaged (PERSEO) and non-wiggler-averaged (MEDUSA1D) simulation codes, and a three-dimensional non-wiggler-averaged (MEDUSA) formulation. These models are compared for examples describing both SASE and MOPA configurations in one dimension, in steady-state, and time-dependent simulations. Remarkable agreement is found between PERSEO and MEDUSA1D for the evolution of the fundamental and harmonics. In addition, three-dimensional correction factors have been included in the MEDUSA1D and PERSEO, which show reasonable agreement with MEDUSA for a sample MOPA in steady-state and time-dependent simulations. © *2008 American Institute of Physics*. [DOI: 10.1063/1.3040689]



- Comparison between MEDUSA & PERSEO was quite good.
- The KMR orbit analysis and application of slippage once per wiggler period worked for these parameters.

COMPARISONS

The JAERI experiment has the longest wavelength and lowest energy so that the amount of slippage relative to the wiggler period is the greatest.

	JAERI oscillator	Jefferson Lab oscillator	BNL/SDL MOPA/SASE	LCLS SASE
Wavelength	22 μm	1.6 μm	0.8 μm	1.5 Å
Bunch Duration, τ_b	17 psec	390 fsec	2.5 psec	74 fsec
Slippage Time, τ_{slip}	3.8 psec	160 fsec	686 fsec	2 fsec
τ_{slip}/τ_b	0.2	0.4	0.27	0.03
$l_c/\lambda_w\,(= \lambda L_G/\lambda_w^2)$	1.8×10^{-2}	3.7×10^{-4}	2.8×10^{-4}	4.4×10^{-5}
$N_w l_c/\lambda_w$	0.93	1.1×10^{-2}	7.3×10^{-2}	5.3×10^{-3}

We find empirically that we must require that $N_w l_c << \lambda_w$ in order for the case where slippage is applied once per wiggler period to work.

SUMMARY & DISCUSSION

- OPC is a powerful tool for modeling resonators.
  - Can treat complex resonator designs with different out-coupling schemes (hole, transmissive, edge), misalignments, distortion
  - Dispersive elements within the resonator will be included in the future.
  - Can propagate the field outside the resonator.

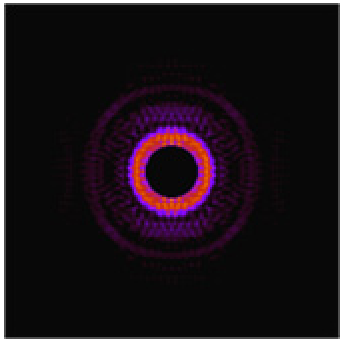
- MEDUSA/OPC has been compared with the 10-kW Upgrade Experiment at Jefferson Lab with good agreement. This represents a full 4-D simulation.
  - Output power in simulation and the experiment are in close agreement.
  - Width and shape of the cavity tuning curve in simulation are in good agreement with the experiment.
  - The average spot size on the mirrors is in good agreement with the experiment.

- GENESIS/OPC and MEDUSA/OPC have been compared for parameters consistent with the JAERI FEL.
  - Steady-state simulations with/without distortion show reasonable agreement.
  - Time-dependent simulations with GENESIS/OPC were not possible because of the magnitude of slippage.
    - Need $N_w l_c << \lambda_w$
    - Difficult to model long wavelength FELs (λ > 20 μm, THz) driven by rf linacs with orbit average formulations.
    - Need to study this issue for a wider range of parameters.

SUPPLEMENTAL VIEWGRAPHS

OPTICAL PROPAGATION CODE (OPC)

ν



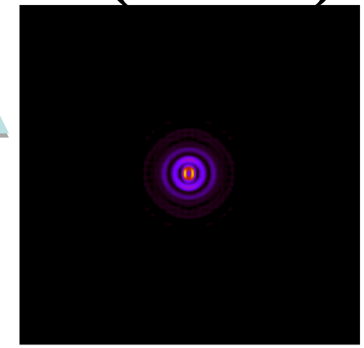
ξ

Input plane

propagation over distance z

paraxial approximation

y



x

Output plane

SPECTRAL METHOD

analytical propagation over z

$$I(\nu,\xi) \xrightarrow{F} I(k_x,k_y) \longrightarrow I'(k_x,k_y) \xrightarrow{F^{-1}} I'(x,y)$$

FRESNEL DIFFRACTION INTEGRAL

$$\iint I(\xi,\upsilon)K(x-\xi,y-\upsilon)d\xi d\upsilon = I(x,y)$$

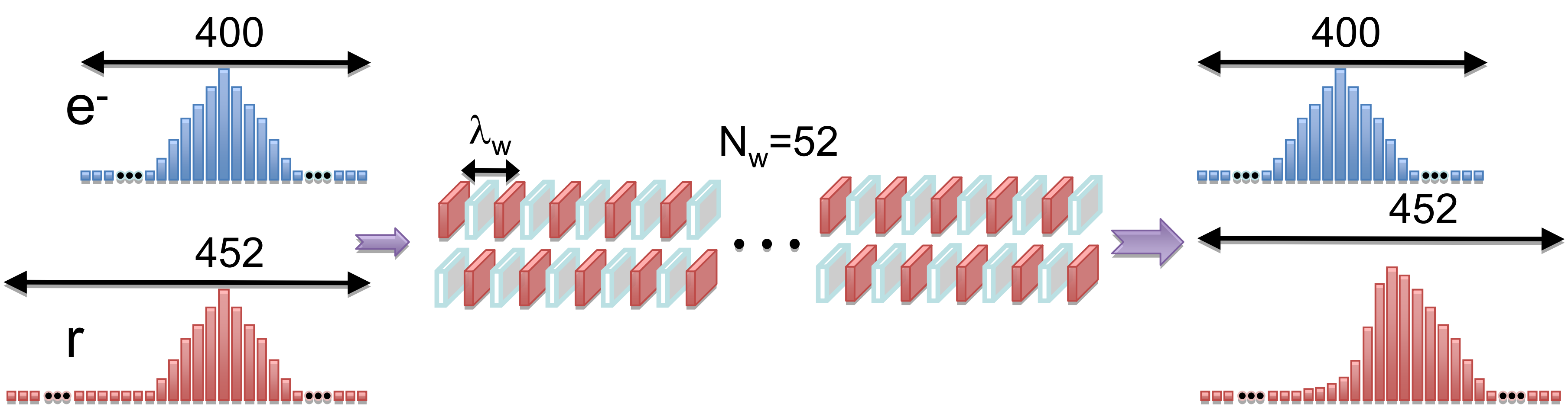
$$I(\nu,\xi)\otimes K(x,\xi,y,\nu) \xrightarrow{F} I(k_x,k_y) \text{ ´ } K(x,y,k_x,k_y) \xrightarrow{F^{-1}} I'(x,y)$$

MEDUSA PROPERTIES

- Fully 3-D
- E&M fields treated using the polychromatic SVEA approximation
  - Time-dependent and/or polychromatic physics
  - Modal decomposition of the fields
  - Amplifier/Oscillator
- Particle dynamics are treated from first principles (not KMR)
  - Harmonics & sidebands implicitly included in orbit dynamics
- Can easily add of new features for Engineering Design Evaluation
  - New wiggler models
    - For example, an APPLE wiggler that can be configured for planar or helical symmetry
    - Input from a field map
  - New beam models
    - Non-Gaussian distributions

GENESIS PROPERTIES

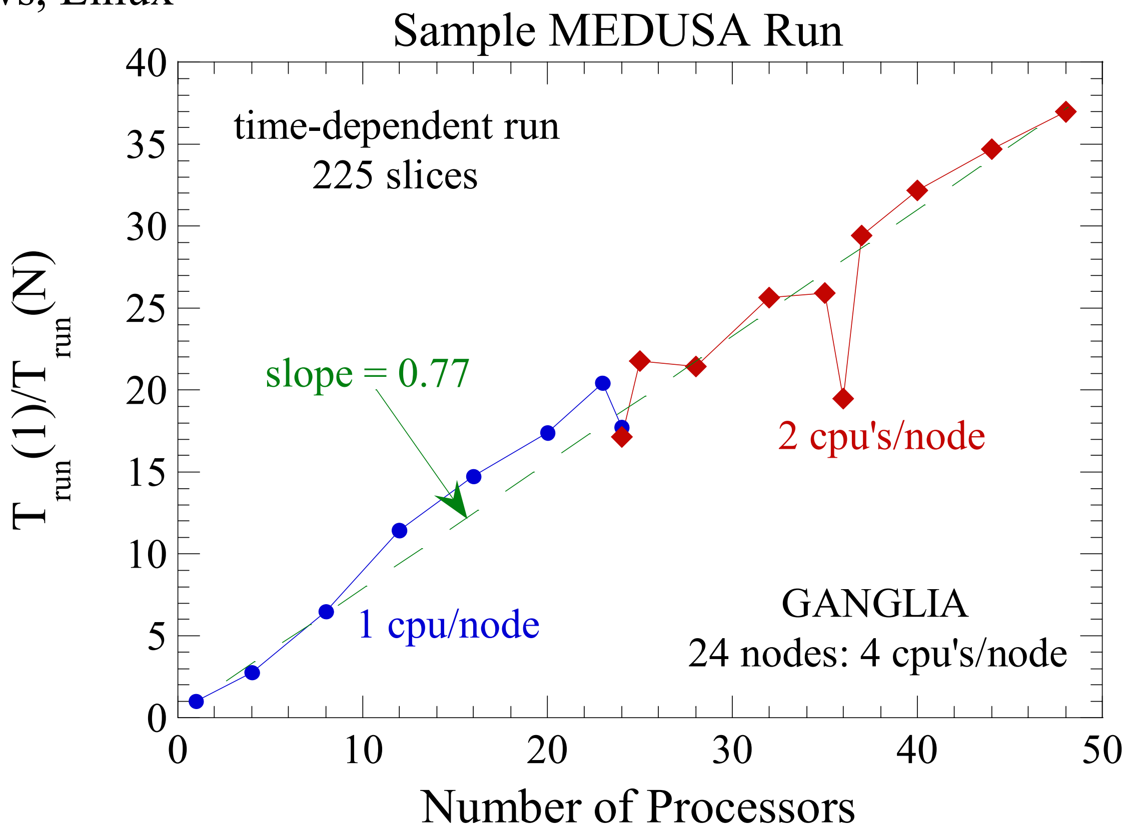
- Solves eikonal field equation
  - slow varying amplitude
- Field discretized on fully Cartesian grid
  - steady- state simulation requires only transverse grid
- Fully 6 dimensional tracking of electron beam
  - equations of motion averaged over undulator period
- Runs in steady-state, time-dependent and scan mode
- External input of magnetic lattice, electron distribution and seeding radiation pulse



PARALLELIZATION

- All elements of MEDUSA/OPC & GENESIS/OPC are parallelized using the Message Passing Interface and Fortran 90
    - MEDUSA
    - GENESIS
    - OPC
    - HERMES (translator OPC → MEDUSA)
- Transportable: Macintosh, Windows, Linux

- Run times vary, but a single pass for the Jefferson Laboratory 10-kW Upgrade experiment requires about 3-5 minutes using MEDUSA/OPC on a Mac Pro using 4 CPU's
    - reasonable
    - faster on a large cluster and depends on the type of interconnect



SLIPPAGE ALGORITHM: GENESIS

- Optical field and electron beam is sampled at intervals (slices)
  - Electron beam slice width = 1 ponderomotive period
  - In following we assume separation between slices = 1 wavelength
- Slippage is implemented by replacing the radiation field with the time slice behind it
  - At end of each undulator period the optical slices are shifted such that the electrons start to interact with the slice slipped in from behind
    - Electron slice interacts with the same optical slice when propagating over a distance of one undulator period
    - If integration step size is less than one undulator period, no slippage is applied until the electron slice has travelled a distance corresponding to one undulator period
  - Slippage allowed is one wavelength per wiggler period, irrespective of operation on- or off- resonance

SLIPPAGE ALGORITHM: MEDUSA

- MEDUSA applies slippage at arbitrary integration intervals [$N_{slip}\Delta z$, $\Delta z << \lambda_w$] by interpolating the power advance between slices.
  - All slices are advanced in parallel over interval [$z \rightarrow z + N_{slip}\Delta z$] between applications of slippage.
  - No change is made in the relative mode amplitudes so that changes in focusing/defocusing from slice to slice is not altered. This is valid as long as:
    - The relative change in the curvature of the phase fronts is negligible over the interval between slippage applications.
    - The separation between slices is small.
  - Slippage is one wavelength per wiggler period only on-resonance. It differs as you go off-resonance [$\propto (\lambda - \lambda_{res})/\lambda_{res}$].
    - MEDUSA takes this difference into account in applying slippage.
- MEDUSA was run subject to slippage applied on every integration step.
  - Fractional slippage applied 30 times per wiggler period in MEDUSA.