Issues and Subtleties in Numerical Modeling of X-Ray FEL's

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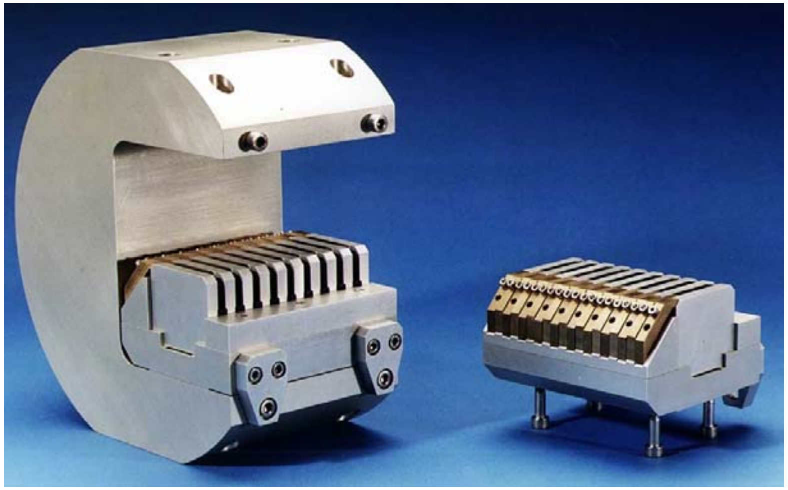
or ...

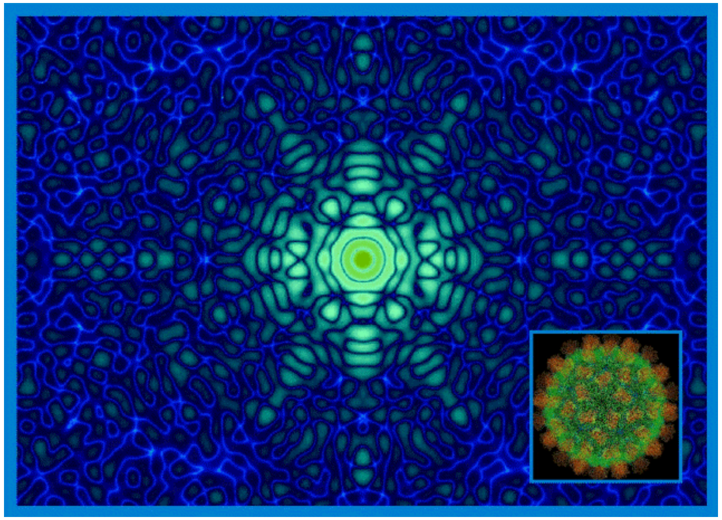
Modeling Big Noise in Hamburg and Palo Alto

Two major, ~quarter-billion-$/Euro, x-ray FEL devices dependent upon noise start-up (*i.e.* SASE) are likely to be built by 2010

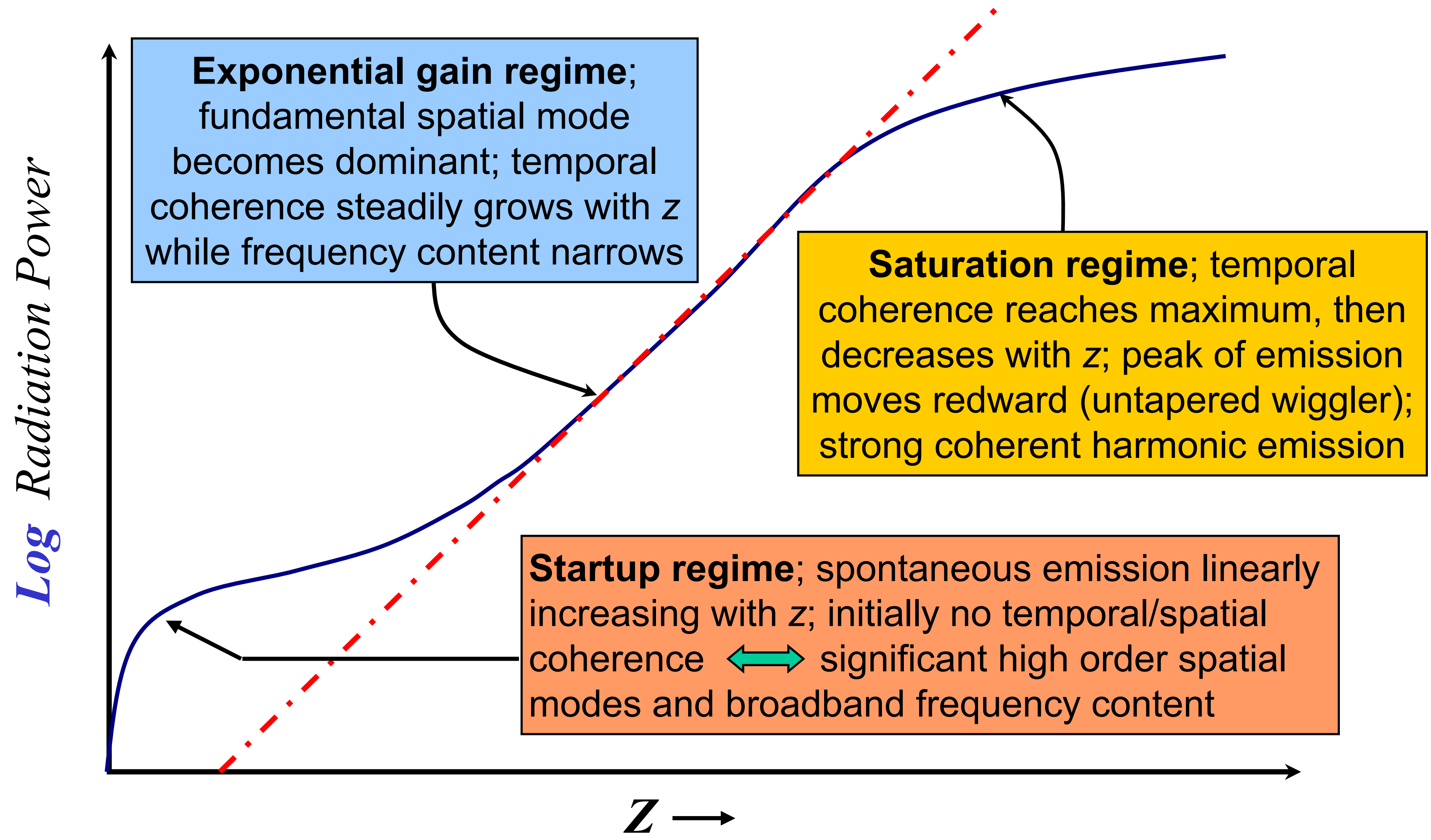
15 GeV Electrons **LCLS** 1.5 Å X-Ray
Linac Coherent Light Source

TESLA





SASE FEL "Topography"



Simulation codes are extensively used to design proposed x-ray FEL's

- Many parameter choices, engineering specifications, *etc*., for these devices have been and will be driven by numerical simulation results
- The underlying simulation codes are non-trivial, both in their algorithms and their software structure

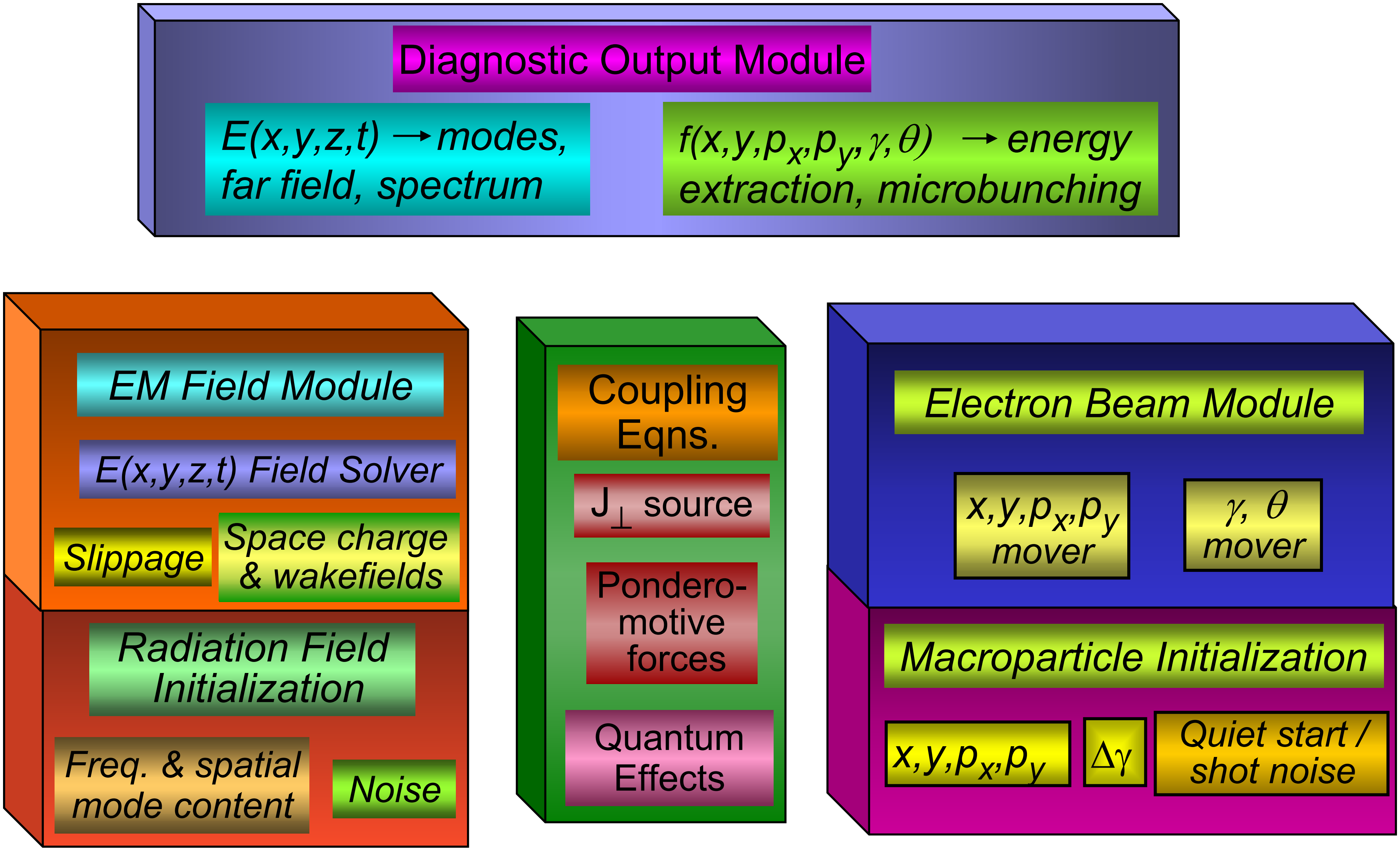
This begs a fundamental, multi-M$ question:

Namely, to what degree of confidence should we believe that these codes are giving dependable answers?

This talk comprise a *personal* selection of topics touching on the confidence issue

- Basic FEL simulation algorithms:
  - SVEA/wiggler-period averaging
  - spatial mode limitations
- Spontaneous emission/SASE start-up:
  - macroparticle shot noise algorithms / harmonics
  - comparison theory/code predictions
  - transition from start-up to exponential growth regime
- Experimental/simulation code interface:
  - LEUTL/GINGER
  - TTF-FEL/FAST3D
  - VISA/GENESIS

Building blocks of a typical FEL code



To model x-ray FELs, a code must make several approximations to be practical

- Eikonal approximation (aka SVEA) :
  - Radiation gain length, synchrotron wavelength, diffraction, refraction, space charge scale lengths >> λ_s ("slow variation")
  - "Fast" time / z variation occurs within a relatively narrow bandpass around a central (ω,k) (modes with peak growth)

$$f(\vec{r},z,t) \Rightarrow \widetilde{f}(\vec{r},z,t)\ \exp\ i\left(k_0 z - \omega_0 t\right)$$

  - Hyperbolic EM eqns transformed to parabolic diffusion eqns

- Discrete radial grid ⇨ finite transverse mode number
  - CPU speed, memory sizes limit grid resolution, dimensionality (GINGER – 2.5D, FAST3D&GENESIS – 3D)
  - Disk sizes, network speeds limit diagnostic storage

Standard code approximations cont.

- "Wiggler-period-averaged" source, dynamics equations
  - forward radiation mode dominates
  - small change in $\widetilde{E}$ over one wiggle period
  - equivalent to eikonal approximation in beam frame
- "PIC" representation of e- phase space
  - finite macroparticle number, smoothed source
- "Slippage" applied at discrete *z* intervals
  - discrete temporal zoning ⇨ finite # longitudinal modes
  - numerically-limited frequency bandpass
- Classical approx. ⇨ neglect of quantum effects
  - # photons/mode >> 1
  - recoil effects small: $h\nu \ll \gamma\, m_e c^2$
  - GENESIS includes $\delta\gamma$ increase from incoherent emission

SVEA, wiggler-period averaging place limits on temporal slicing of e-beam, radiation

- Time-domain codes (*e.g.* GINGER, GENESIS, FAST3D) uniformly slice the e-beam & radiation field temporally
- Slippage applied at *discrete* intervals in t,z with

$$\Delta z_{slip} = \lambda_w \times c\Delta t_{slice} / \lambda_0$$

  – Δz_{slip} determines the width of the bandpass window $\Delta\omega$ around the central angular frequency ω_0

  – minimum value for $\Delta z_{slip} = \lambda_w$ ⇨ $\Delta\omega \leq ½\,\omega_0$

  – neither the SVEA nor wiggler-period averaging apply to frequencies near or beyond this value

- For $\Delta z_{slip} / \lambda_w \geq O(4)$ and $L_G / \Delta z_{slip} \geq O(8)$, SVEA and wiggler-period averaging ~ OK for all wavelengths within the bandpass
- ***However***, limited λ bandpass can present other difficulties…

Example of unphysical aliasing + gain suppression due to limited bandpass

LCLS parameters: 14.35 GeV, 3400A, 1.2 mm-mrad, λ_w=3 cm

FODO focusing lattice

K=3.71 chosen to give peak FEL gain at 1.5000 nm

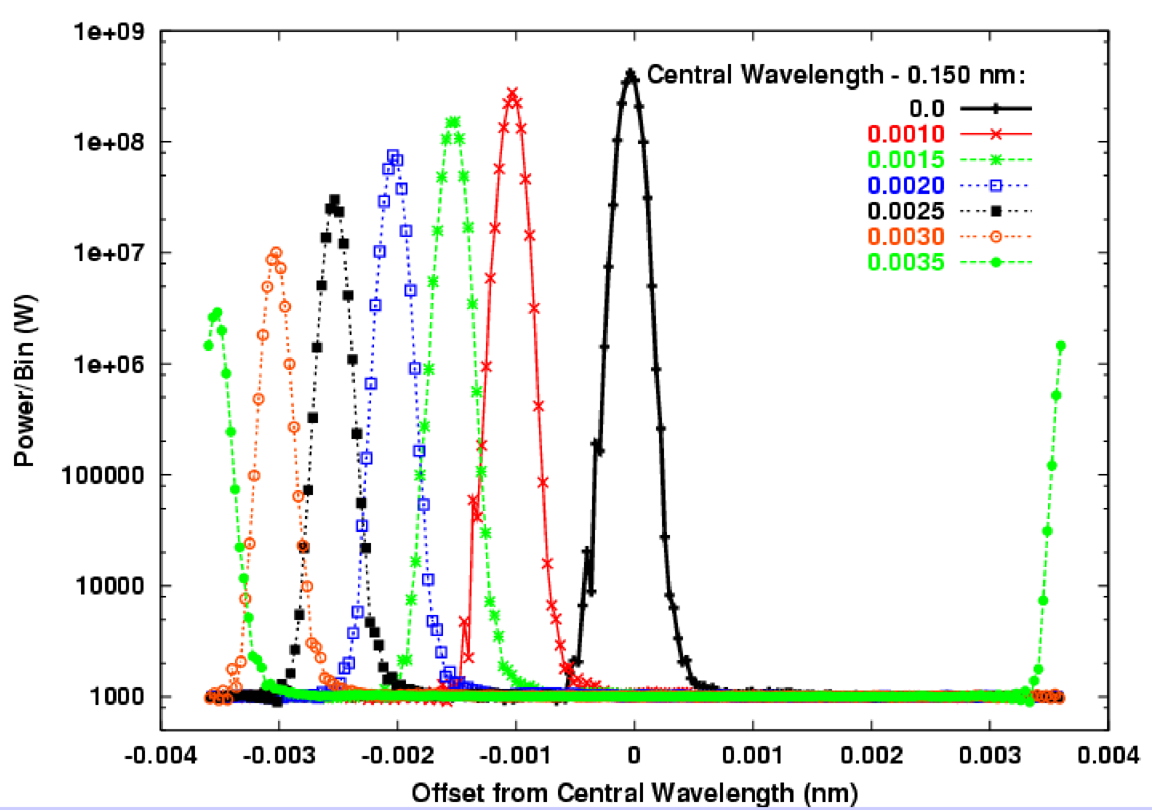
L_{gain} ~ 5.3 m

192 slices in time

Δz_{slip} = 64 cm >> λ_w

Each run initialized with 1.0 kW / frequency bin

Center wavelength of simulation bandpass varied from 1.5000 to 1.5035 nm



Result: Gain unphysically drops by ~1.8X from bandpass center to edge

⇨ caution must be used when simulating e-beam energy chirp

Wiggler-period averaging can break down for higher order spatial modes

- High-order spatial modes (in *r* or *x,y*) have relatively little gain but do suffer significant diffraction:

$$Z_R(M_\perp) \sim Z_R^0 / M_\perp^2$$

- Requiring mode diffraction length > λ_w equivalent to:

$$M_\perp \leq \left(\frac{4\pi\varepsilon}{\lambda_s}\right)^{1/2} \left(\frac{\beta}{4\lambda_w}\right)^{1/2}$$

- For LCLS with β~18 m, $M_{crit} \sim 12$ and one expects few problems for reasonable transverse grid resolution
- For DESY 70-nm with β~1.0 m, $M_{crit} \sim 2.4$ ⇨ possible problems
- For VISA with β~0.27 m, $M_{crit} \sim 1$!!

  ⇨ coupling to "high"-order modes *and* fundamental probably less accurately followed during start-up phase

The Importance of Being Noisey…

- SASE *is* amplified shot noise
- *Ergo*, a code must load noise to be accurate/believable

But

- One need not /*cannot* load all $\sim 10^{10}$ actual beam e-
  - only small frequency portion of noise spectrum becomes amplified, *i.e.* $\Delta\omega/\omega_0 \sim O(\rho) << 1$
  - similarly, causality & limited slippage isolate most temporal slices from one another

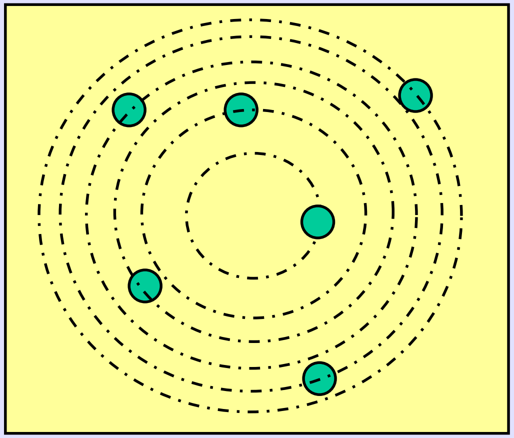
$\sim 10^5$ macroparticles can accurately predict the gross (and most fine) aspects of a SASE FEL from start-up to deep saturation *iff* the noise load algorithm is appropriately clever

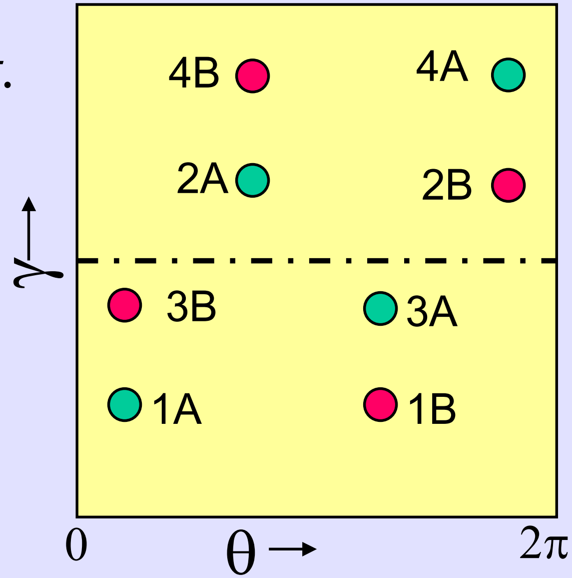
Microbunching loading schemes

- (Presumed) Poisson statistics gives ensemble-averaged properties of moments of $\delta f(\vec{x},\vec{p},\gamma,t)$
- Quiet start (*e.g.* bit-reversal) ⇨ microscopic 6D noise-free distribution with minimal 1st –order correlations between different coordinates
- Most schemes load microbunching noise in *longitudinal position only*
  - δf moment fluctuations in other 5D coordinates weakly couple to bunching, *e.g.*

$$\delta b / b_{shot} \approx \frac{z}{L_g} \frac{8}{N_P} \frac{\Delta\gamma}{\rho\bar{\gamma}}$$

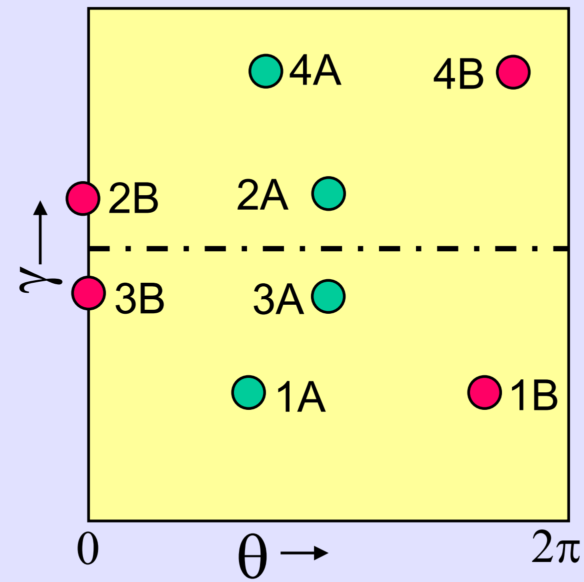
- "Penman-McNeil" like-scheme:
  - $\delta\theta$ assigned *independent* of 5D position
  - extension: "clone" particles at $\theta_i + \pi$
- Litvinenko scheme: e-,e+ pair at same 6D location, $\delta\theta$ separation produces bunching





Variation in β_z ➡ possible harmonic problems

- β_z variation ($\delta\gamma$, ε) can cause *unphysical* microbunching even in a *drifting* beam
  - partial suppression (Penman-McNeil scheme) by greater clone #
  - FAST3D applies "striping" correction to global (γ,θ) distribution to eliminate $<(\gamma_0-\gamma_i)^n\,\theta_i>$ correlations
  - higher harmonics most sensitive



Later in z: Without clones, very strong bunching at fundamental; with clones, fundamental suppressed but strong bunching at cos 2θ

- In strong gain regime, bunching at harmonic *m* coupled to (*m±1*)
  - *2m+1* clones at same β_z needed to obtain proper growth of harmonic *m*
  - 8-fold symmetry needed for 3rd harmonic

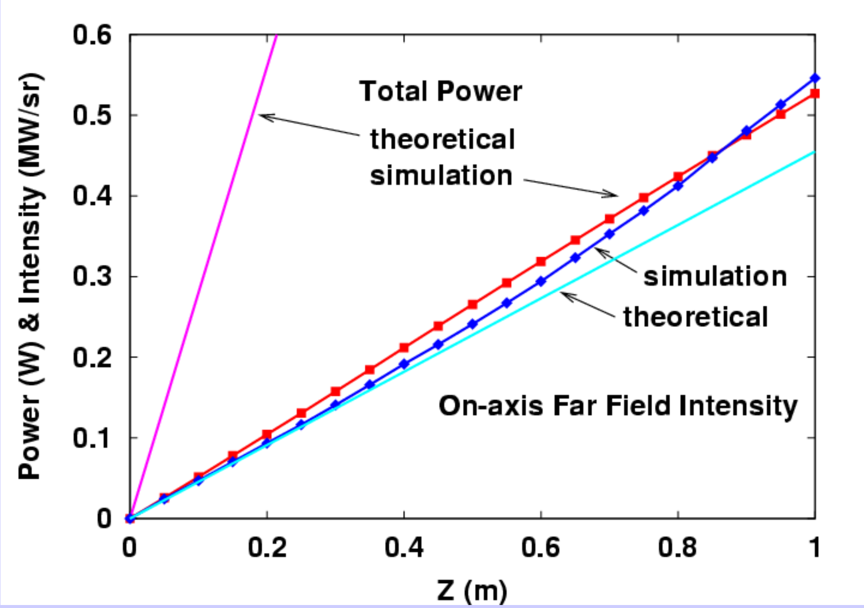
Beamlet loading scheme…

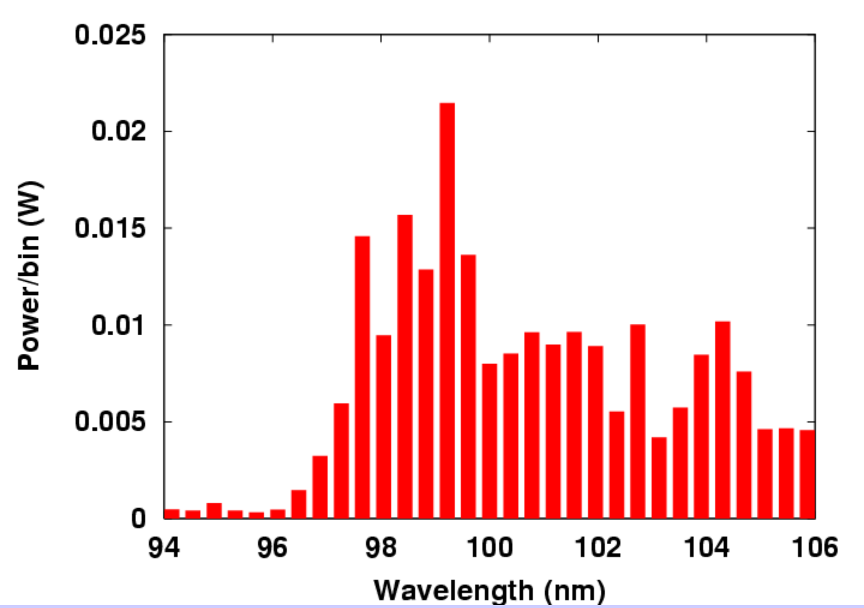
- GINGER, GENESIS divide each temporal slice into many (~128-2048) individual beamlets,
  - each beamlet has unique initial 5D coordinate (x, y, p_x, p_y, γ)
  - each has $2M$ members, each with identical 5D coordinate
  - members loaded in θ with uniform separation of π/M ; $\Rightarrow$ zero bunching for drifting beam through harmonics *1-M*
- For GINGER,
  - SASE harmonics important (cascades, multi-λ_w undulators)
  - noise microbunching $\delta\theta$ distribution determined *individually* for ***each*** beamlet *j* (see paper in July PRST-AB)
  - $\delta\theta_{ij}$ composed of sum of complex phasors over harmonics *1-M*,
  - each beamlet harmonic follows negative exponential distribution

❖ Note: effective # for shot noise statistics = # e- in *total Δt interval* between adjacent slices, *not in just one wavelength*

GINGER simulation of spontaneous emission in the very low gain regime

Parameters: I_B=1.0 A, γ=500, λ_s=100 nm, ε_n=1 π mm-mrad ($4\pi\varepsilon/\lambda_s$ = 0.25), λ_w=2.5 cm, K=1.414, $\Delta z_{slip} = \lambda_w$, 2048 macroparticles/slice*256 slices*8 runs



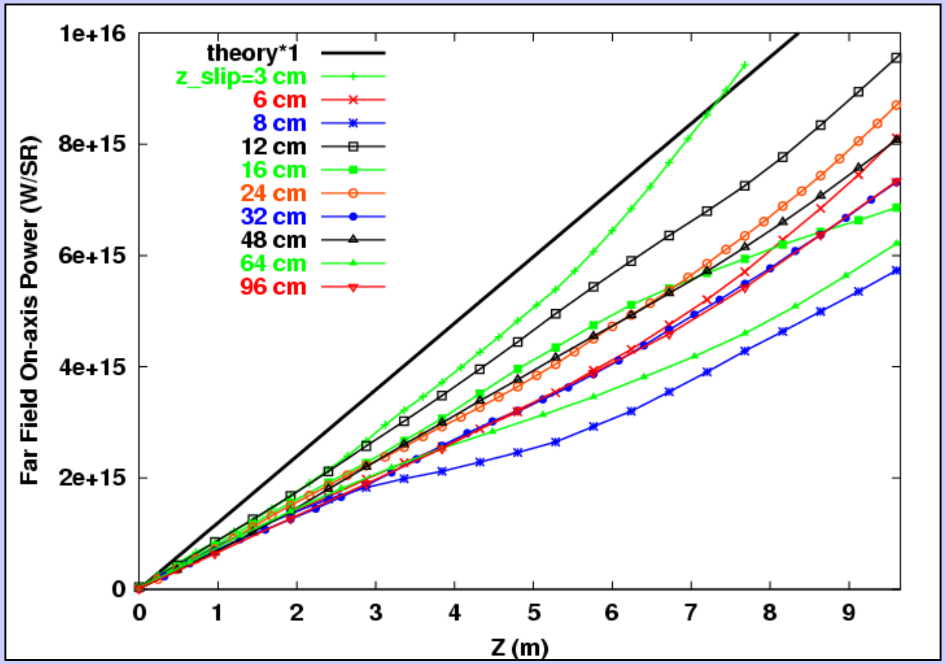


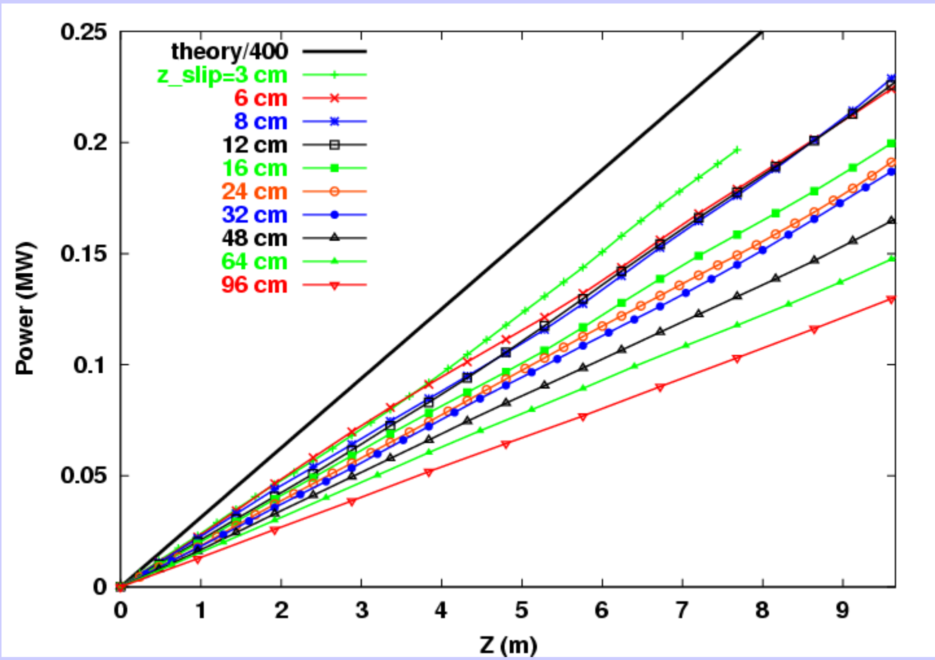
- Excellent agreement in far field intensity
- 5X discrepancy in total power

- 0.19 W near-field power integrated over ±4% bandpass agrees with 0.21 W theory prediction

GINGER Simulation of Spontaneous Emission Startup in LCLS

Parameters: std. LCLS --- 3400A, 14.35 GeV, 1.2 mm-mrad, 0.15 nm, K=3.71, $4\pi\varepsilon/\lambda_s$= 3.6; scan of spontaneous emission sensitivity to Δz_{slip}





far field intensity results:
- generally agrees within ~25%
- some sensitivity to $\Delta z_{slip} \equiv$ bandpass

total power results:
- >400X discrepancy theory/sim.
- stronger sensitivity to Δz_{slip}

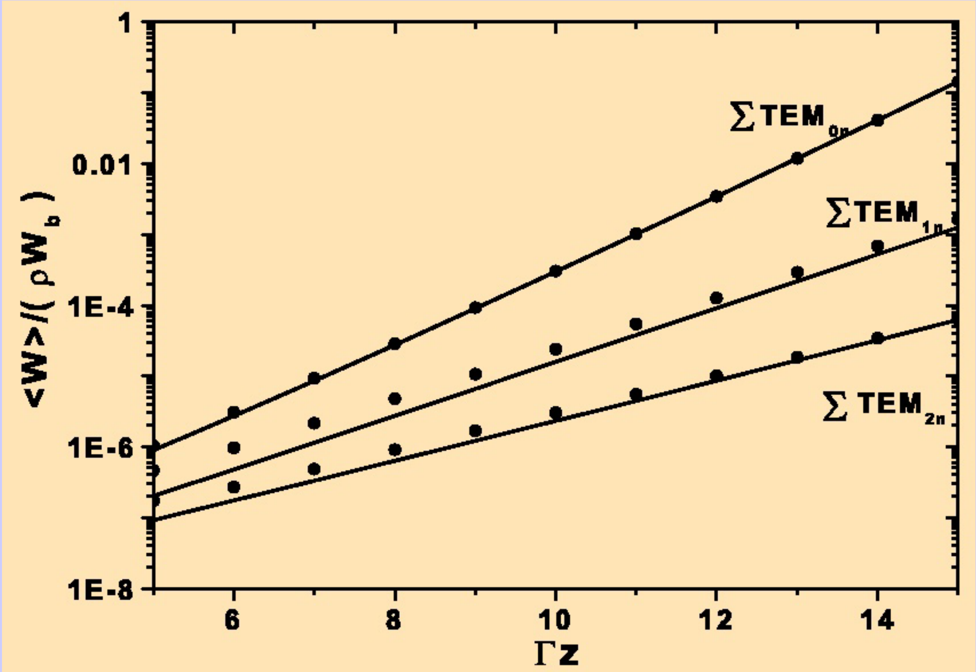
High order, non-axisymetric modes quite important in total power emission

Linear FAST simulation, analytic results show contribution of high order modes

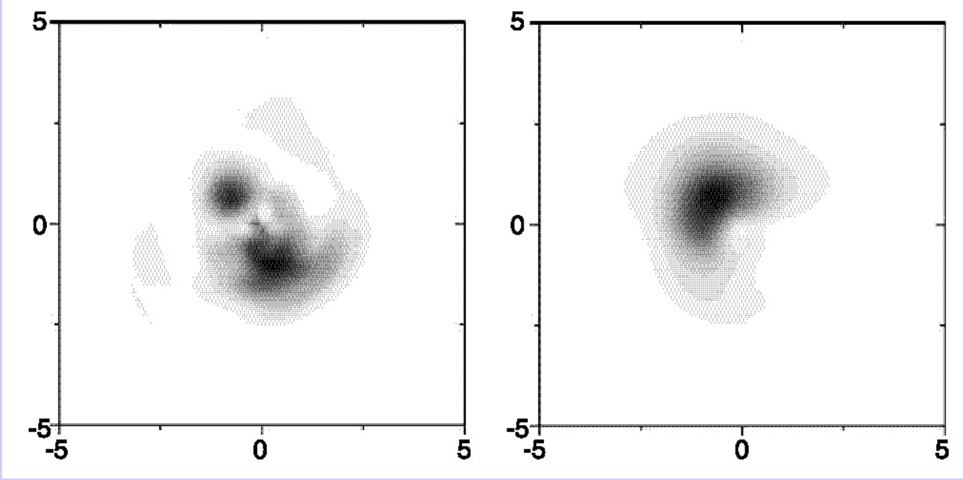
Results from Saldin *et al.*, *Opt. Comm*. 186 (2000), 1895.

- no energy spread or emittance, $L_G/Z_R=1$, 7 x 10^7 e- / λ_s
- 3D linearized code FAST

Radiation power vs *z* in gain lengths for 3 lowest azimuthal modes (each again summed over lowest 3 radial modes); lines=*theory*; dots=*simulation*



Transverse radiation profiles across 1 temporal radiation slice at z/L_G=5 and 10



Courtesy M. Yurkov

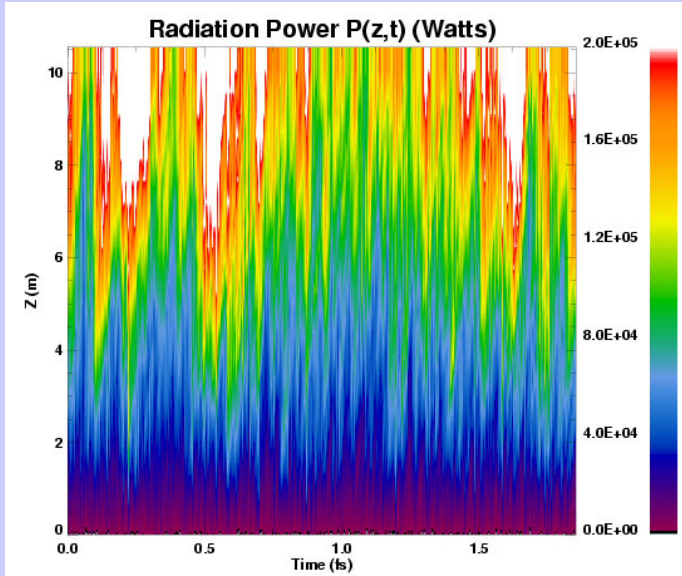
GINGER "standard" LCLS example of noise -> organized start-up -> exponential gain

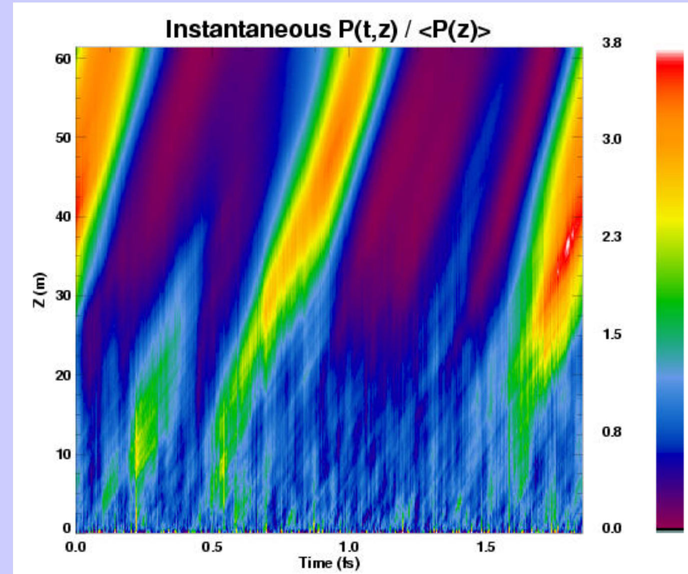
Total power shows development into spikes by z~10 m

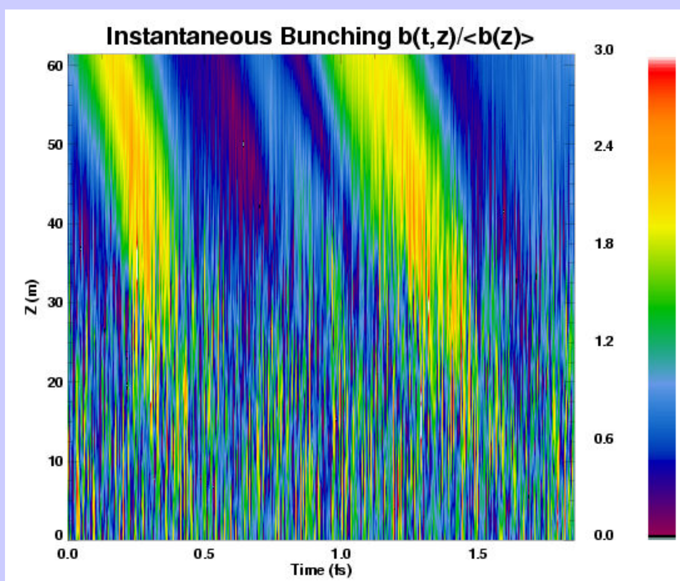
Normalized power shows self-similar spike propagation $[c - v_G] \sim 2/3\ v_{slip}$

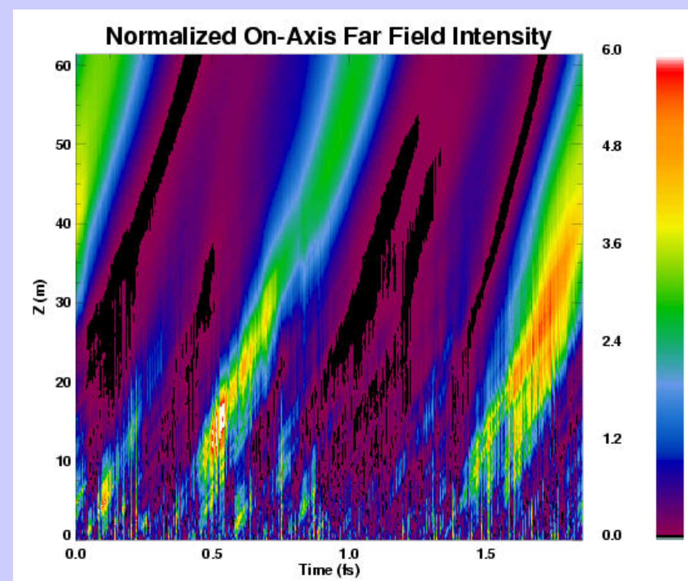
On-axis far field radiation sub-*c* spike propagation evident earlier in z

Norm. bunching shows self-similar spike propagation at $v_G > \langle v_z \rangle$



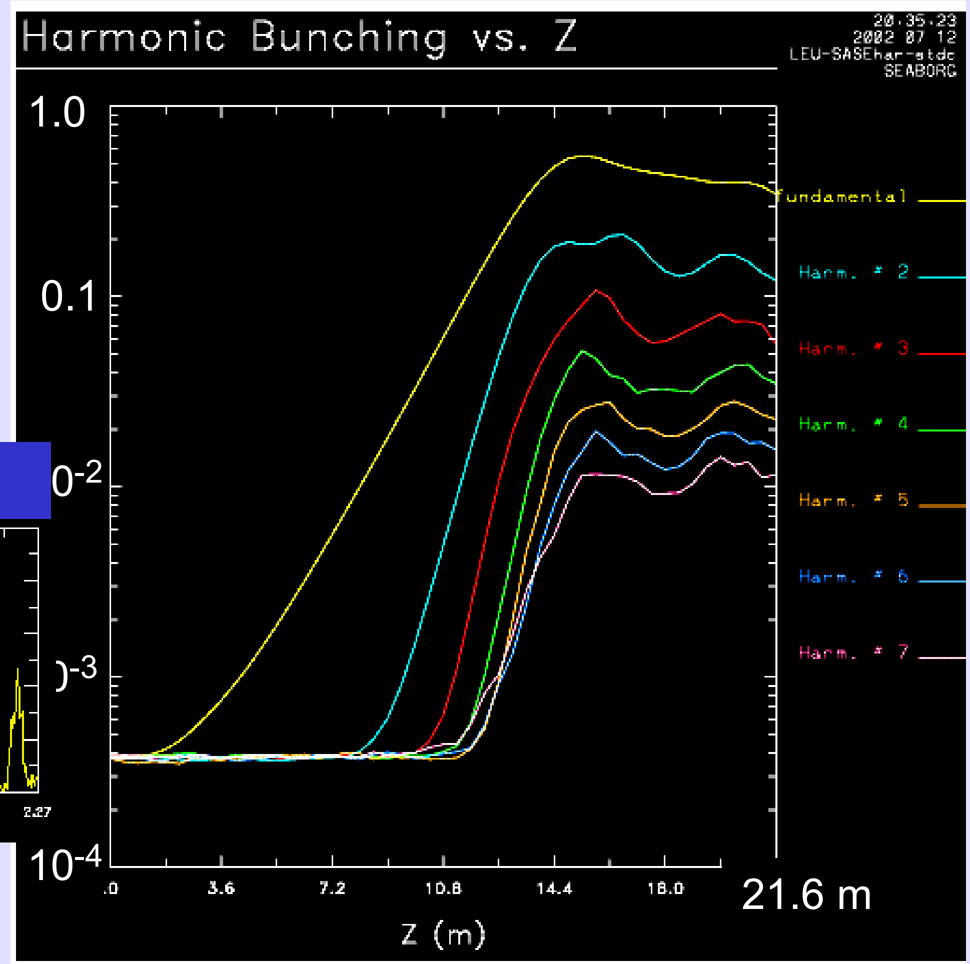




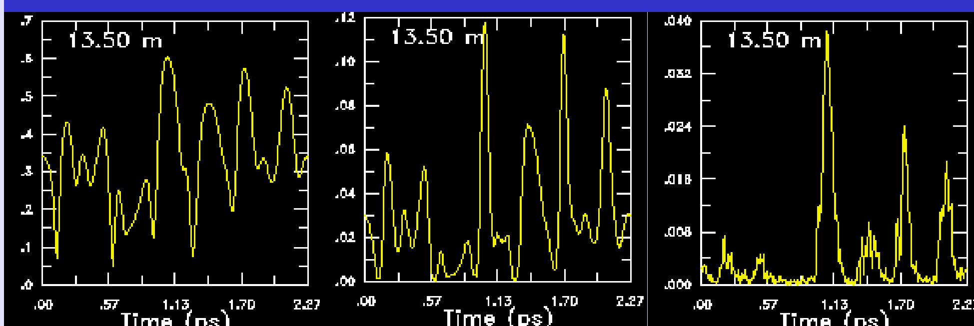


Nonlinear harmonic growth in the SASE regime – GINGER / LEUTL example

<u>Sim. parameters</u>: 5π mm-mrad, 150 A, 519 nm, 219.5 MeV, $\Delta\gamma$=0.43, ρ ~ 2.1 x 10^{-3} ; 32768 macroparticles/slice x 384 slices; 150 CPU hours split over 64 IBM-SP4 processsors



Fundamental b1, b3 and b5 at z=13.5m



Bunching "snapshots" just before saturation show usual spikiness; spike width in b_3, b_5 narrower but not by 3,5 fold

Highlights of 3 simulation/expt. efforts

(1) LEUTL/GINGER (2) TTF-FEL/FAST3D (3) VISA/GENESIS

- Common features:
  - Beam compressor ⇨ complicated 5D phase space
  - Short pulse effects important
  - Pulse-to-pulse machine repeatibility fair-to-poor
- Common prediction successes:
  - L_{gain}, P_{sat}, z_{sat}
  - θ_{FWHM}
  - E_{pulse}, pulse-to-pulse output statistics (TTF, VISA)
  - Harmonic content (LEUTL, VISA)

GINGER modeling of APS LEUTL results

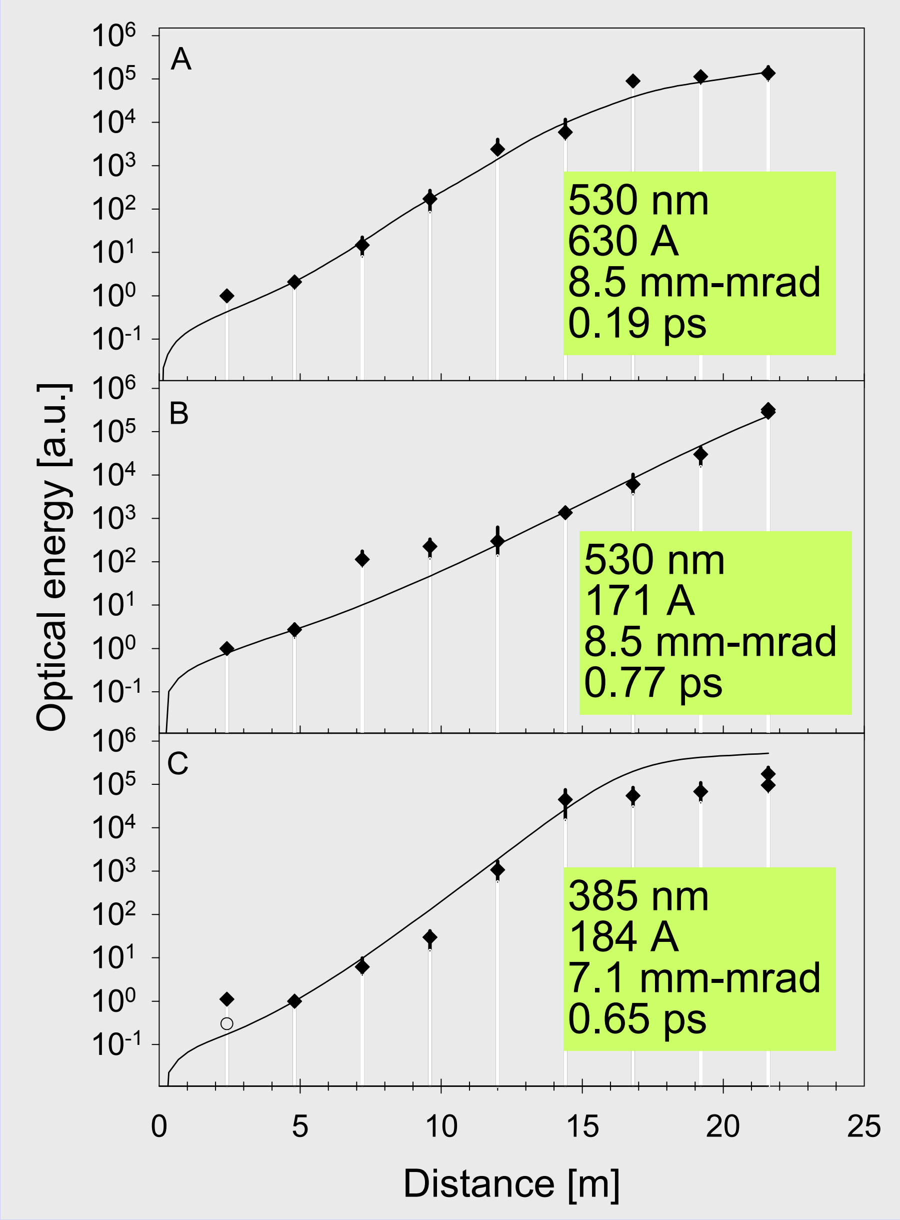
LEUTL Experiment:

beam charge~0.3 nc
each dot =100 shots
error bar 25-75th percentile

Pulse length in Case B purposely increased to prevent saturation

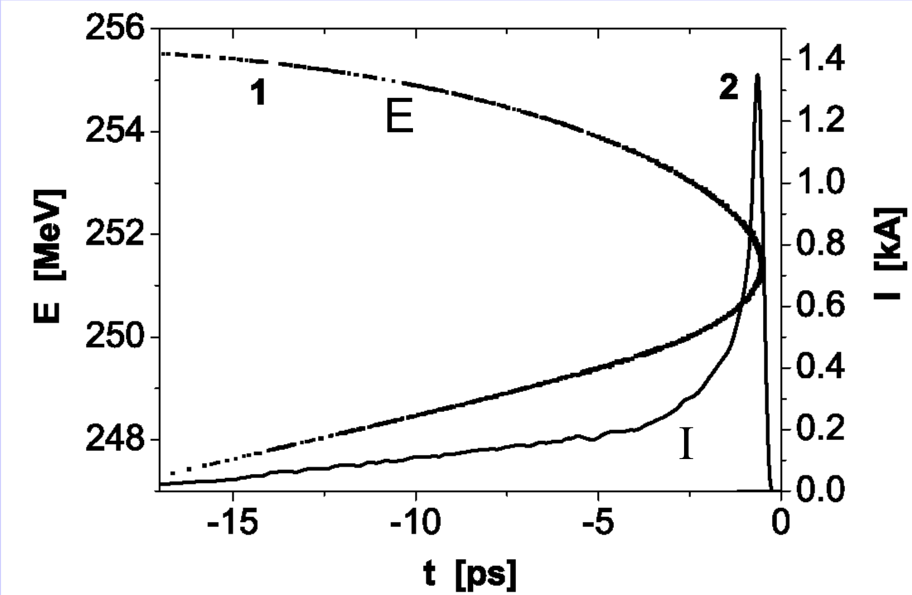
GINGER Simulation:

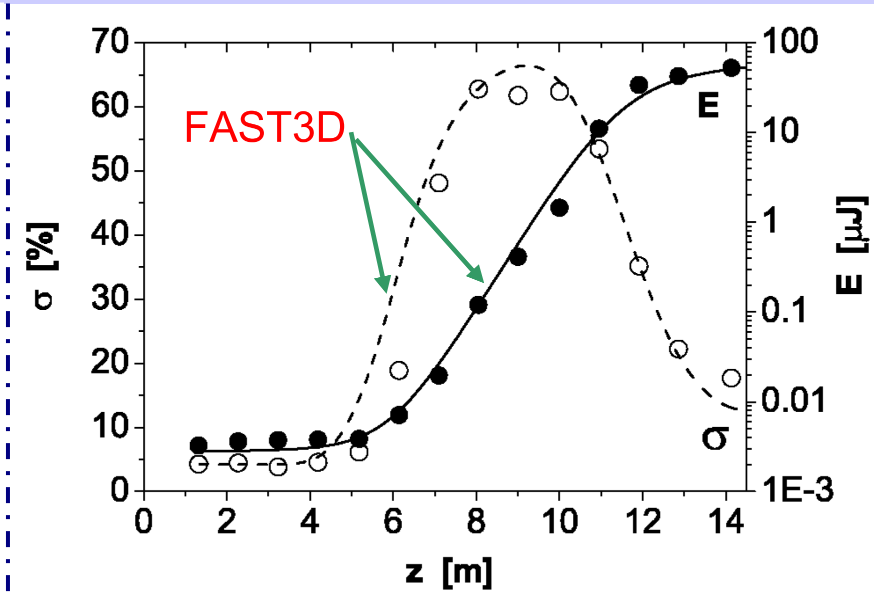
- simple Gaussian 5D distributions
- energy spread σ slightly adjusted from nominal value for better fit
- output energy normalized for exact overlap at z=5 m
- each solid line = 50 GINGER short pulse SASE runs with different random # seeds



Courtesy Z. Huang - APS

FAST3D modeling of 100-nm TTF-FEL





Results published in Ayvazyan *et al.*, PRL, **88**, 104802 (11 Mar 02)

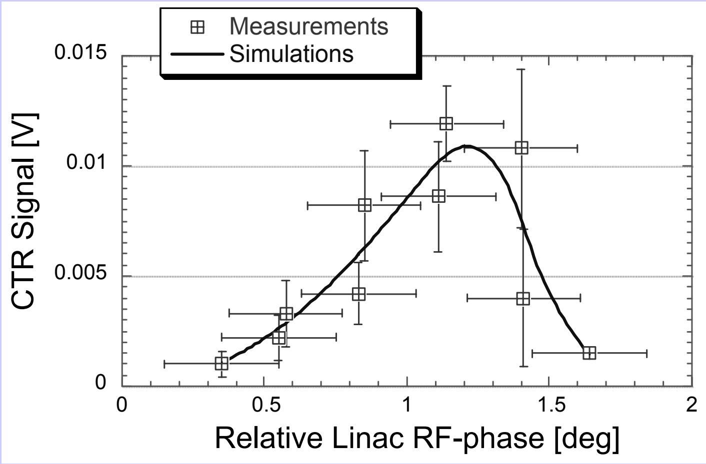
- Key conclusion is emission comes from 1.3-kA current spike produced by bunch compressor (VISA-like)
- Experimental measurement of L_G, output power fluctuations, spectral width gives independent value for I_B, τ_p, ρ
- FAST3D modelers found excellent agreement (including angular distribution) using I_B =1.3 kA, Gaussian profile with FWHM=120 fs, δE=100 KeV, ε = 6π mm-mrad

VISA electron beam properties reconstructed and input to GENESIS code

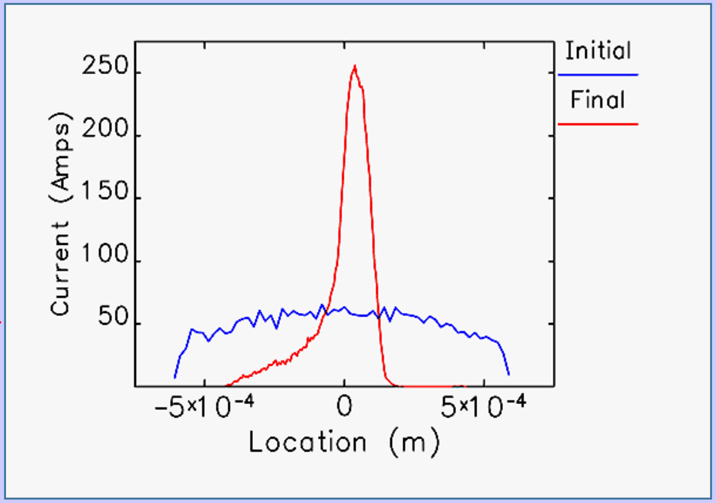
Beam Parameters at Undulator Entrance

Energy	71 MeV
Spread	0.1 %
Peak Current	250 A
Emittance (projected)	2.3 mm·mrad
Undulator period	1.8 cm
Undulator parameter	0.88
Wavelength	850 nm

Bunch Length at Undulator



Predicted Current Profile



PARMELA + ELEGANT injector to undulator simulation

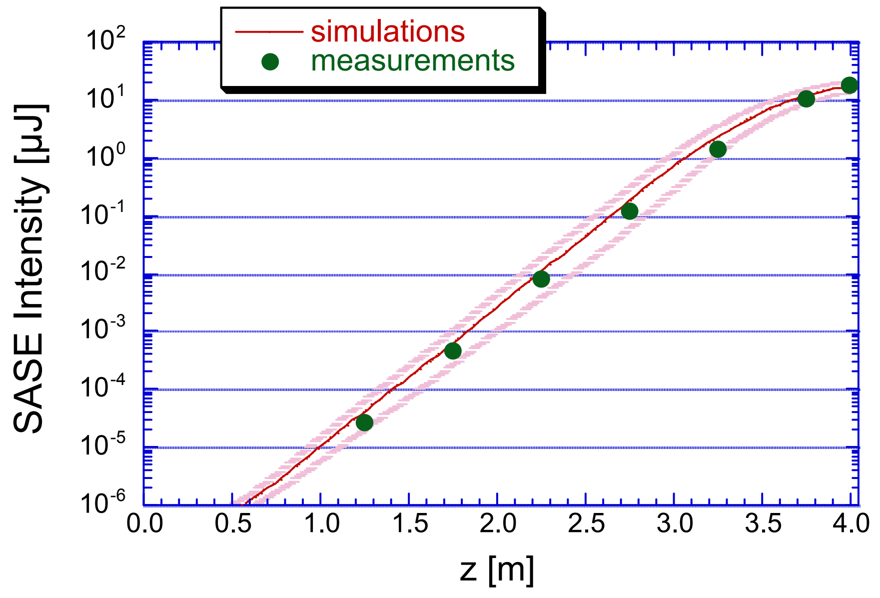
Courtesy S. Reiche - UCLA

Comparison of GENESIS simulation and VISA experimental results

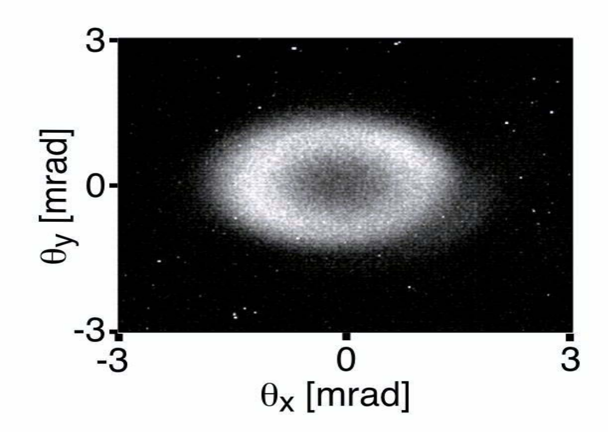
GENESIS simulation shows excellent agreement with experimental results:

- Power growth (including saturation)
- Spectrum + bandwidth (*not shown here*)
- (Fluctuations – insufficient # sim. runs)

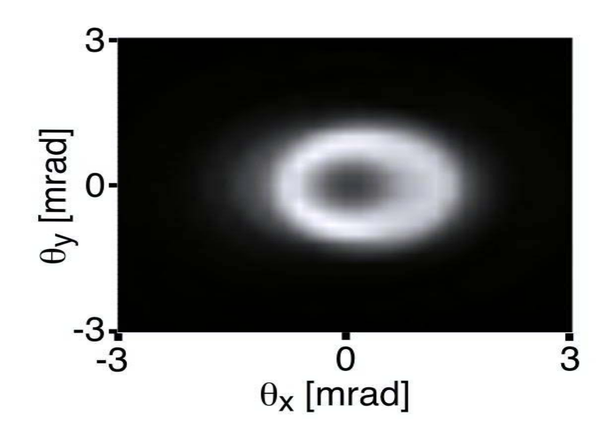
- Near & far field spatial mode distribution



Far Field (Measurement)



Far Field (Simulation)



Courtesy S. Reiche - UCLA

Different individuals will have differing perspectives on the present robustness of x-ray FEL modeling

- From microwave to infrared to far UV wavelengths, simulation codes have had good success in reproducing gain lengths, effective start-up and saturation power, far field angle, *etc.*, for SASE-based FEL's
- A critical factor is good knowledge of beam parameters, including 6D phase space
- Undoubtedly, there will be some surprises in the 4- to 0.15-nm region
- However, funding decisions often also have a surprisingly random component…

Different individuals will have differing perspectives on the robustness of x-ray FEL modeling

APS control room, 22 July 2002

The author thanks the following individuals for multiple discussions and contribution of results:

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Heinz-Dieter Nuhn

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