What you always wanted to have from a simulation software (and you never dare to ask for)

October 4th 2016

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SLAC National Accelerator Laboratory
Linac Coherent Light Source

SOS WORKSHOP 2016

ESRF The European Synchrotron

Elettra Sincrotrone Trieste

U.S. DEPARTMENT OF ENERGY

Office of Science

Stanford University

SLAC NATIONAL ACCELERATOR LABORATORY

DISCLAIMER

Shadow has been, and, somehow, still is, the beamline designer best friend!

During my talk, any sentences/comment on Shadow, that could sound like diminishing the value of Shadow, is not intended neither wanted.

All my personal gratitude for the great effort Franco (Cerrina) and Manuel (Sanchez del Rio) put on making Shadow available for the entire community, and, for the support provided!

Shadow is still the most user friendly and one of the most valuable program for Optic Simulation!

And with the new interface, it’s even better!

And, whatever I will say today, is based on my personal experience only and is not meant to be a teaching lecture

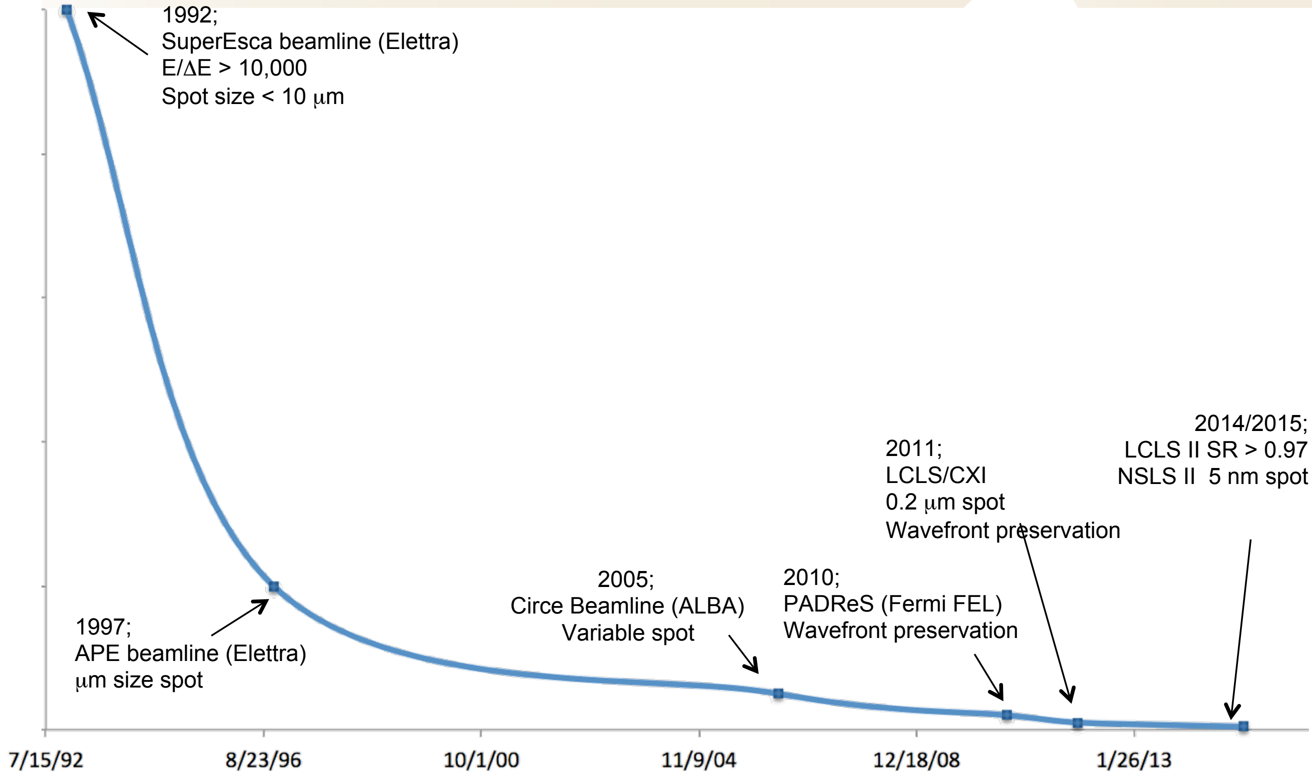
Credits

Examples, pictures and results shown in this presentation has been obtained using the following software:

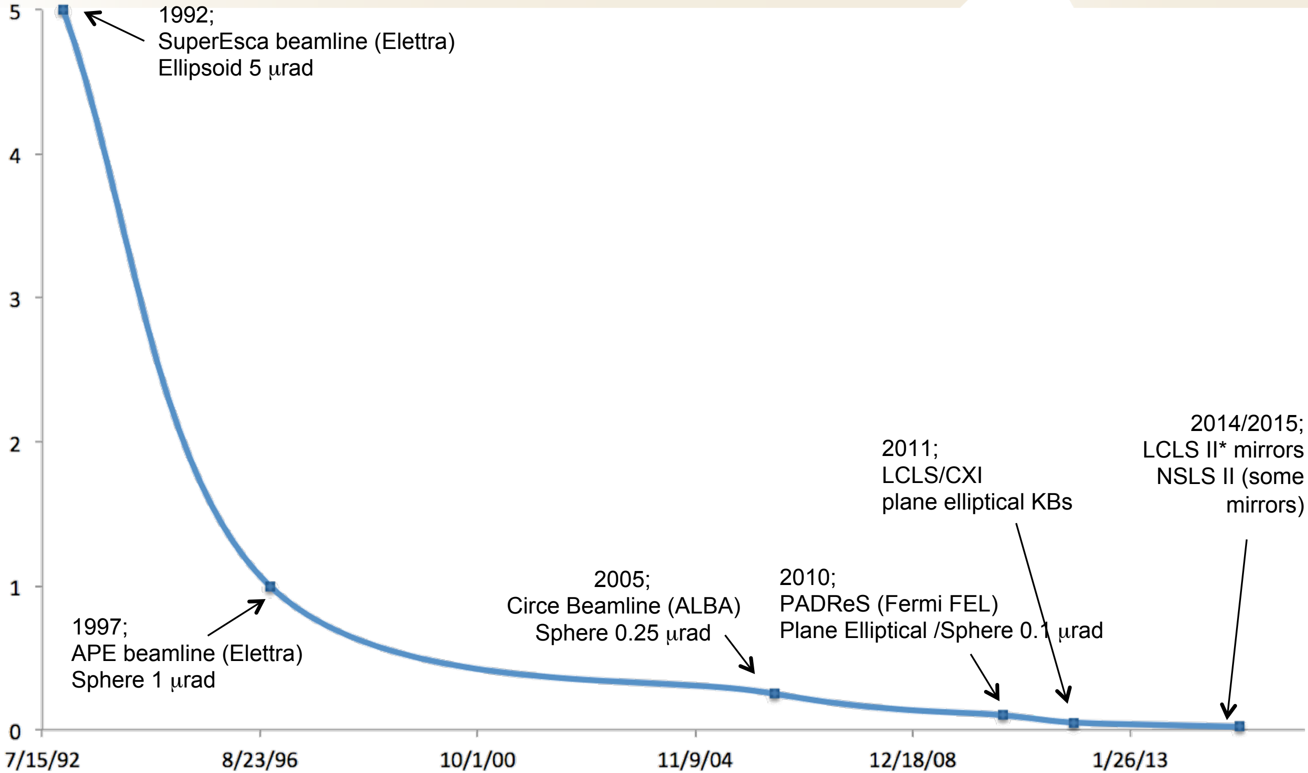
- SHADOW
  - *F. Cerrina and M. Sanchez del Rio "Ray Tracing of X-Ray Optical Systems" Ch. 35 in Handbook of Optics (volume V, 3rd ed.)*
- Jacek Krzywinski (SLAC) – Software developed in Matlab using Fourier optics techniques including Fresnel propagator or angular spectrum method to solve propagation of time dependent optical fields through nonhomogeneous media. For certain applications the angular spectrum method allows to go beyond the paraxial approximation.
- Tom Pardini (LLNL) – XFELSim (wavefront propagation)
- Josep Nicolas (SLAC) – Kirchhoff integrals
- Lorenzo Raimondi (Elettra) – WISE
- …and of, course, Excel, MatLab and LabVIEW!

Original (initial) approach

Pushing the envelope - requirements

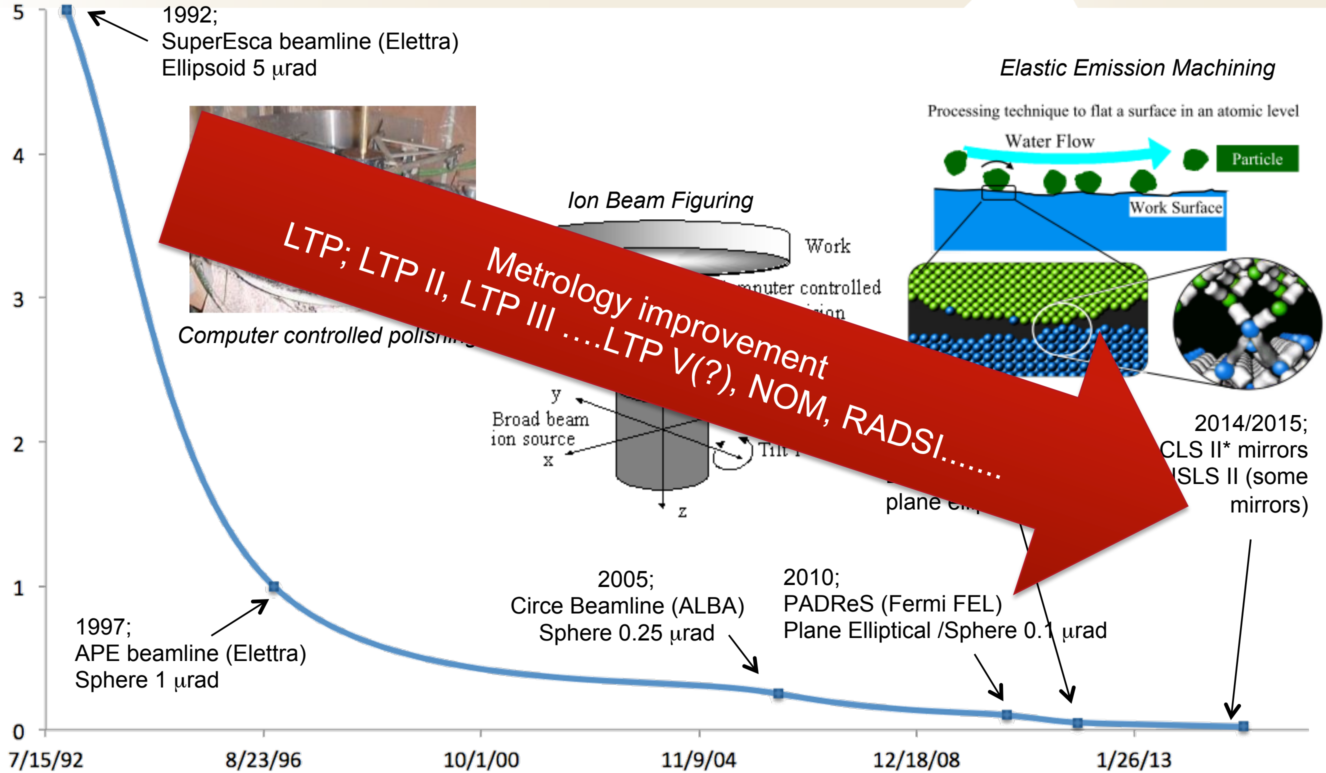


Pushing the envelope - specifications



*LCLS mirrors are specified in height (nm rms).

Pushing the envelope



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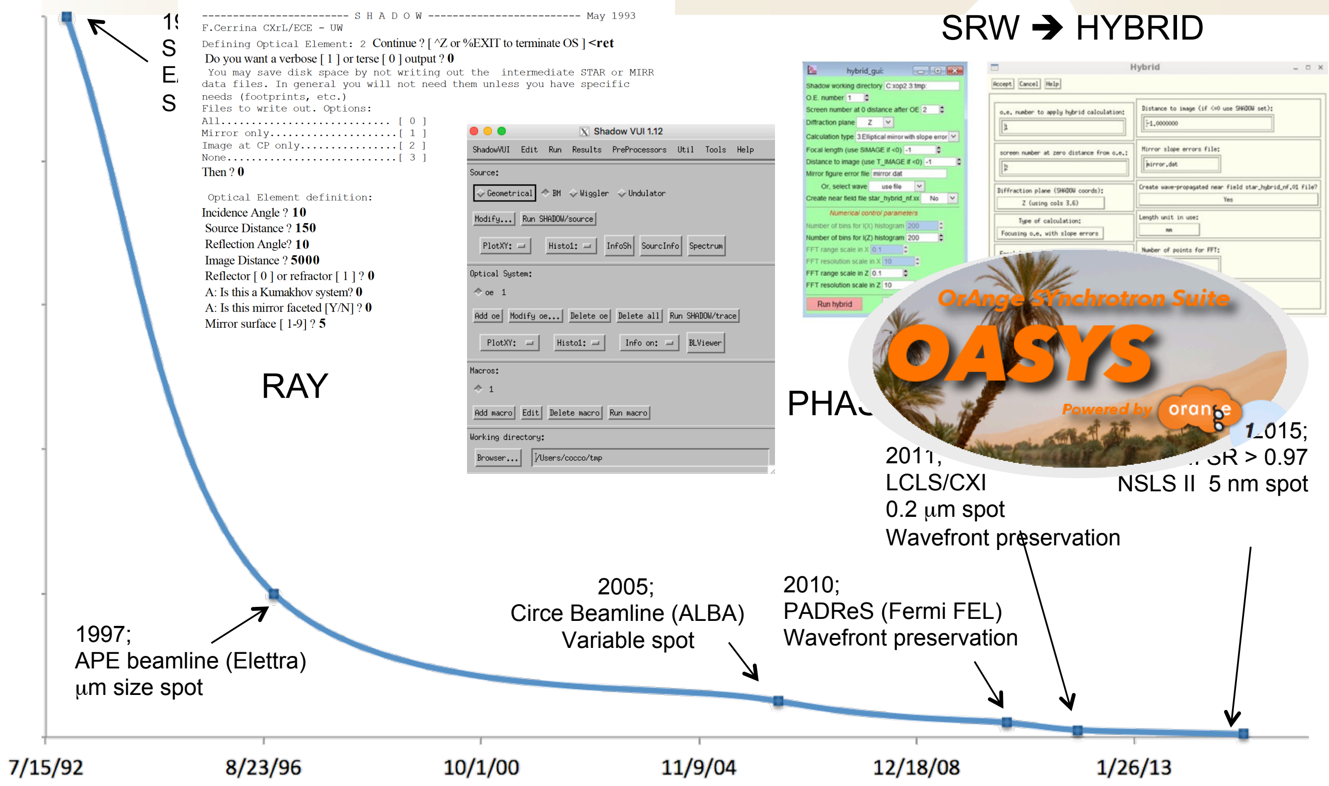
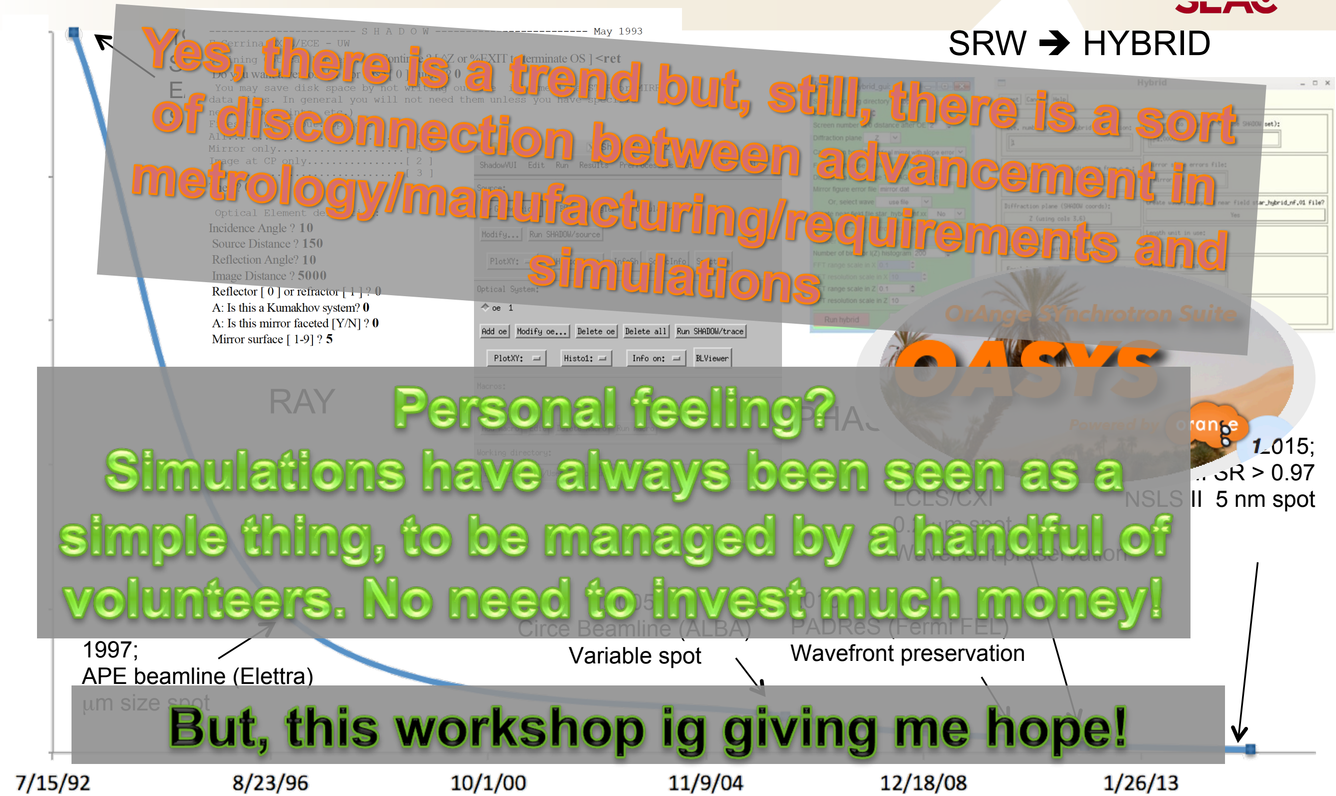
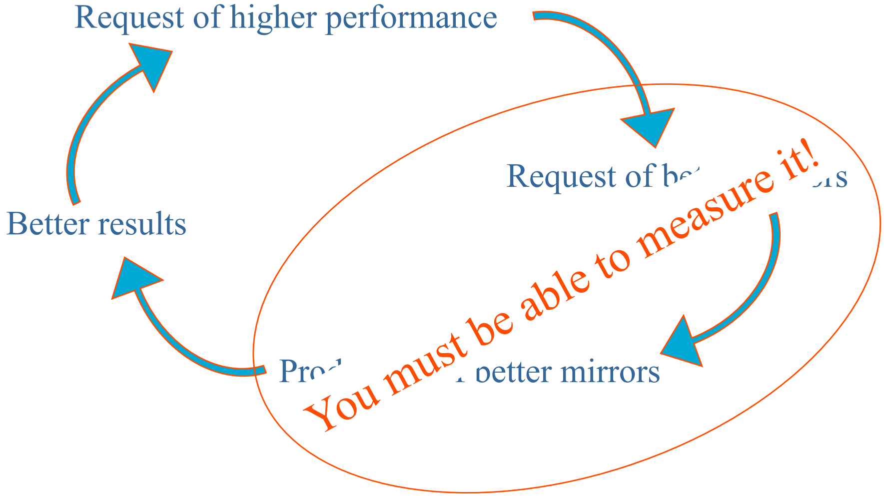
Pushing the envelope – simulation?



Pushing the envelope – simulation?

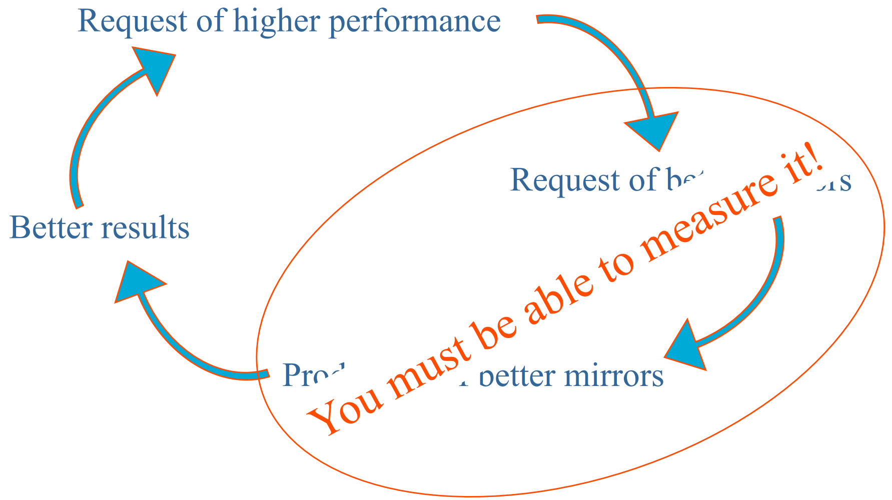


Metrology



COST Action **P 7**
KO meeting
Orsay Sept. 6th 2002

Metrology



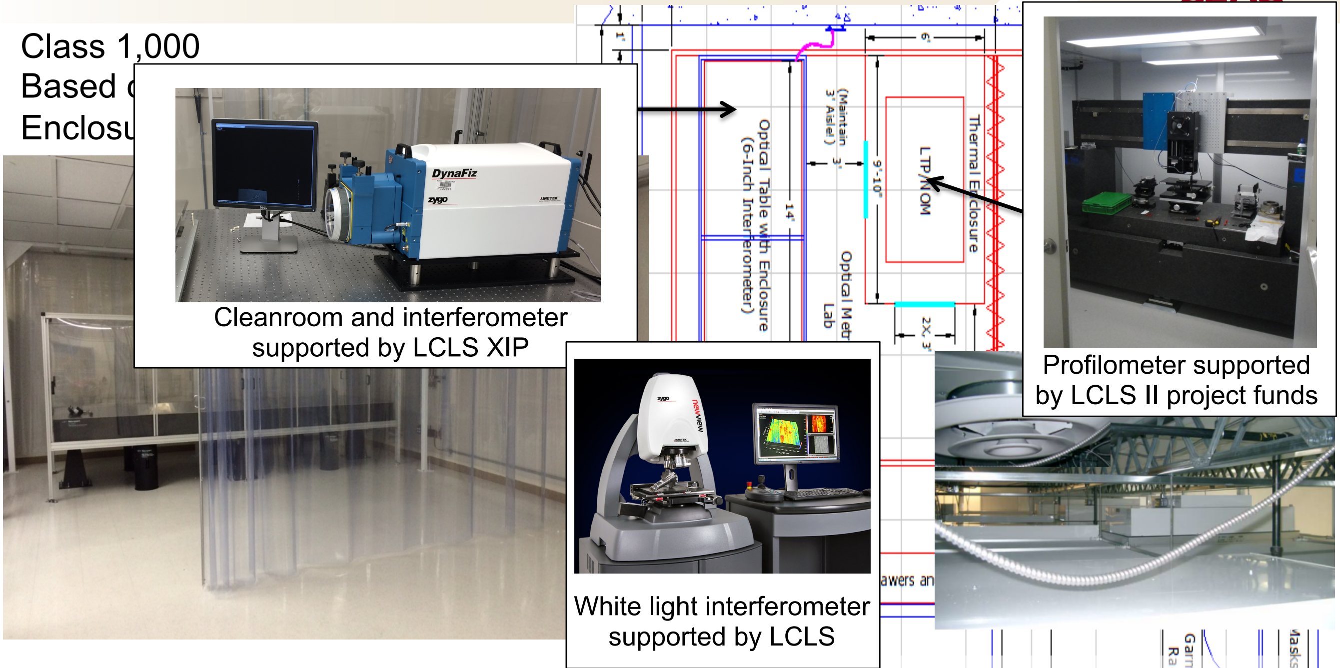
Internal review
Mirror and Metrology
Menlo Park, Feb. 2014

Metrology improvement drove the mirror manufacturing improvement and, ultimately, push the science forefront limits*

**….ok… it's a bit of a stretch…*

SLAC, for the first time in 50 years, has a metrology Lab.

Class 1,000
Based c
Enclosu



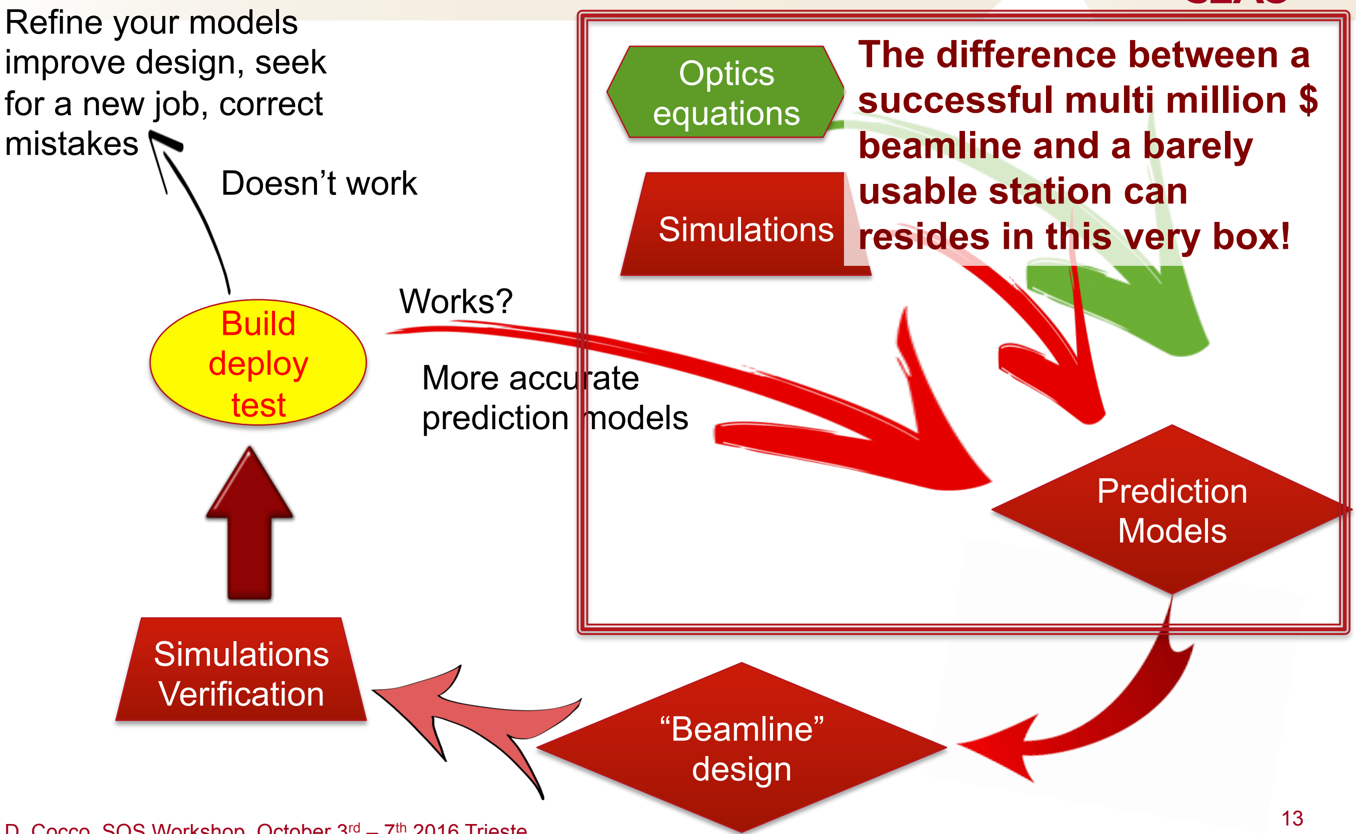
Cleanroom and interferometer supported by LCLS XIP

Profilometer supported by LCLS II project funds

White light interferometer supported by LCLS

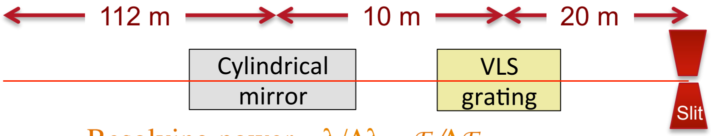
Humidity and temperature controlled by maintaining stable the circulating air.
Temperature stability: +/- 0.5°C with up to 8 people in the room (by design) at 85°F
Humidity: +/- 2.5% at 50%

Simulations



Simulation assisted mistakes

SXR monochromator



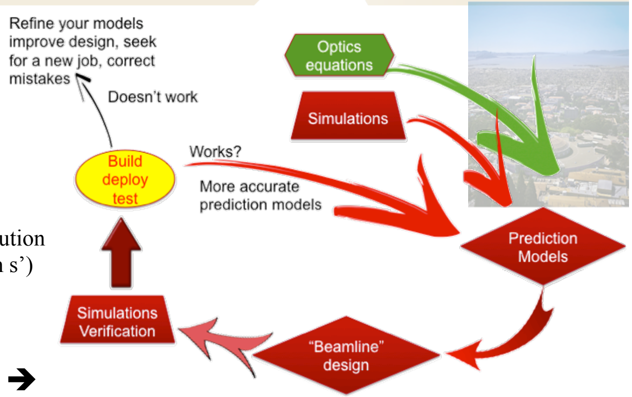
Resolving power $= \lambda/\Delta\lambda = E/\Delta E$

$$\Delta\lambda_{entrance} = \frac{s \cdot \cos(\alpha)}{Nkr} \qquad \Delta\lambda_{exit} = \frac{s' \cdot \cos(\beta)}{Nkr'}$$

Entrance and exit slit contribution (with slope errors included in s')

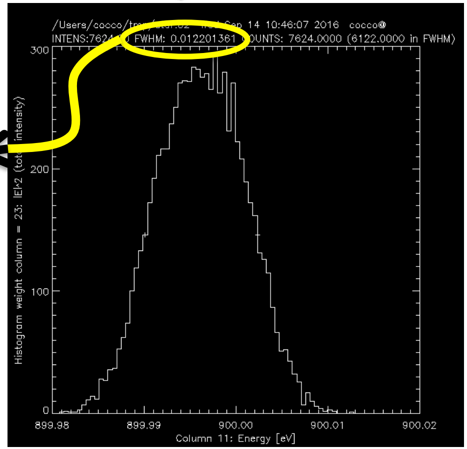
$$\frac{\Delta\lambda}{\lambda} = \frac{\delta d}{d}$$

Groove placing precision contribution



For a 600 l/mm grating, source σ'=10 μrad, σ=27 μm ➔
Calculated resolving power at 900 eV = **73,700**

FWHM = 0.0122 eV
E/ΔE=73,770



Pretty cool but WRONG!

Simulation assisted mistakes

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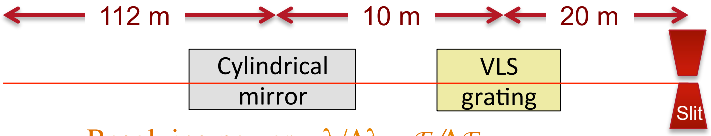

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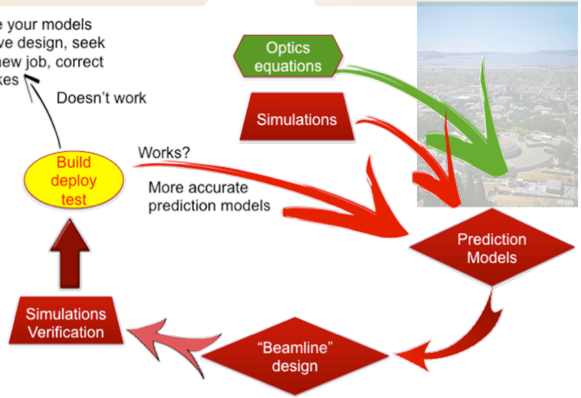
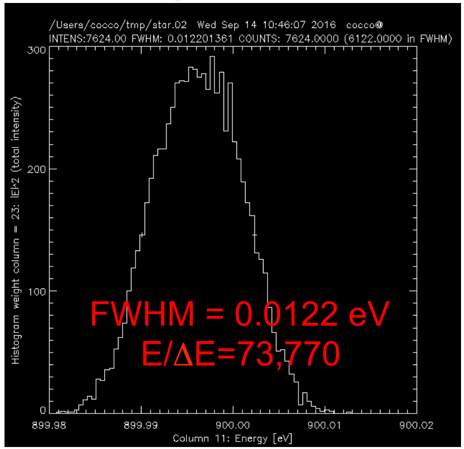
Diffraction limited contribution: ΔE/E = 1/N

N=600(l/mm)*0.01mrad*112m/0.0189rad [α] = 35,500
e.g. ΔE=0.025 eV





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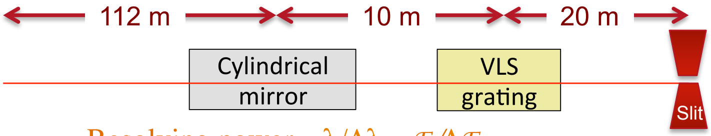

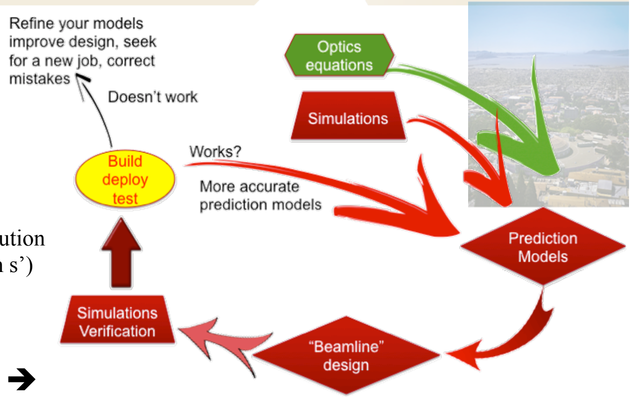

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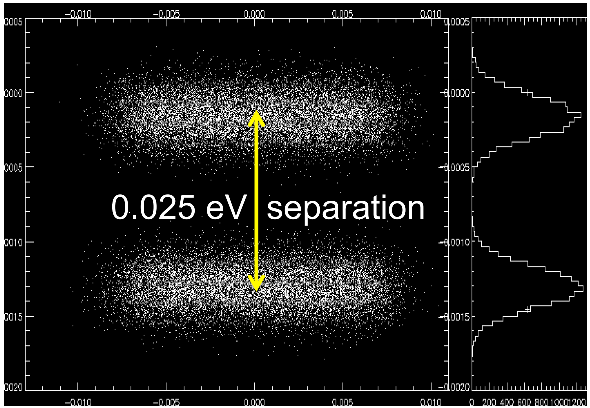
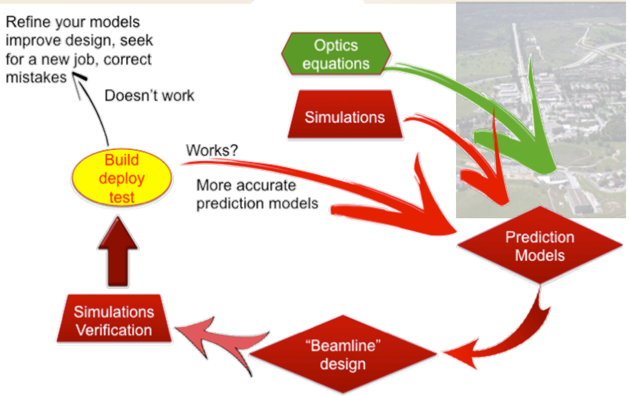


Similarly…..

Exercise:
Estimate and simulate, if needed, the spot size of this beamline and the required mirror specifications!



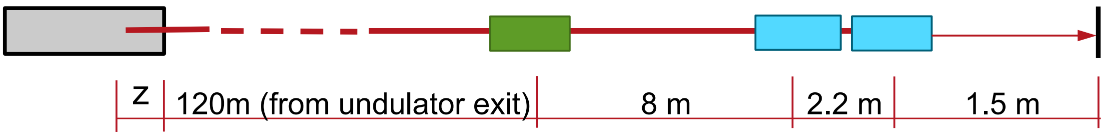
$$s' = \sqrt{\delta_{dif}^2 + \delta_D^2 + \delta_{\sigma rms}^2}$$

δ_{dif} = diffraction limited spot

δ_M = source limited (s'/s=r'/r)

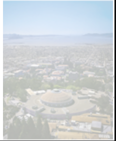
$\delta_{\sigma rms}$ = slope errors contribution

At which extent, is this correct?



Shape and not slope

Specification of glancing- and normal-incidence x-ray mirrors



Eugene L. Church, FELLOW SPIE
Peter Z. Takacs, MEMBER SPIE
Brookhaven National Laboratory
Upton, New York 11973

System coherence length (W)

$$W = \frac{\sqrt{2}\lambda}{\Theta \sin\vartheta}$$

Angular radius ($1/e^2$)

In a diffraction limited optics:

$$\Theta = \frac{\lambda}{L\sin\vartheta} \qquad W \approx \sqrt{2}L$$

Effect of slope errors on the performance of mirrors for x-ray free electron laser applications

Tom Pardini,[1,*] Daniele Cocco,[2] and Stefan P. Hau-Riege[1]
[1]*Lawrence Livermore National Laboratory, Livermore, California 94550, USA*
[2]*SLAC National Accelerator Laboratory, Menlo Park, California 94566, USA*

$$\frac{I(0)}{I_0(0)} = 1 - \frac{8}{\Theta^2}\mu_{\mathrm{rms}}^2 - \left(\frac{4\pi}{\lambda}\cos\theta_i\right)^2 \sigma_{\mathrm{rms}}^2$$

Intensity in focus (Strehl Ratio)

$$\mu_{\mathrm{rms}}^2 = (2\pi)^2 \int_{1/L}^{1/W} df_x \mathrm{PSD}(|f_x)f_x^2$$

Slope errors contribution

$$\sigma_{\mathrm{rms}}^2 = \int_{1/W}^{1/\lambda} df_x \mathrm{PSD}(f_x)$$

Surface finishing contribution

In a diffraction-limited optic, with W > L (classical FEL cases), only shape errors are important and slope errors, in principle, does not play any role in spot enlargement or beam inhomogeneity

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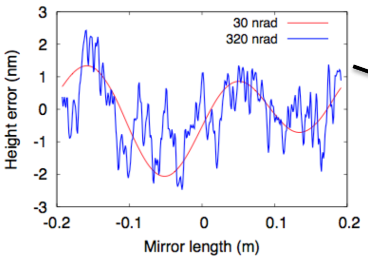
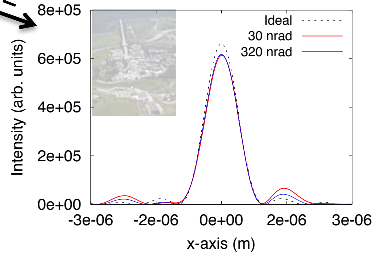


W > L



In a diffraction-limited optic, W > L (Mirror length)

Effect of slope errors on the performance of mirrors for x-ray free electron laser applications

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Ordering (procuring) a 30 or 300 nrad slope error mirrors does not make any difference

Simulations tell you this, only if you ask the right question!

In a diffraction-limited optic, with W> L (classical FEL cases), only shape errors are important and slope errors, in principle, does not play any role in spot enlargement or beam inhomogeneity

But slope can be important

Specification of glancing- and normal-incidence x-ray mirrors

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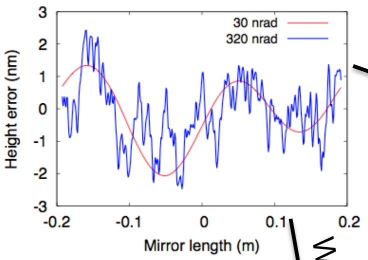
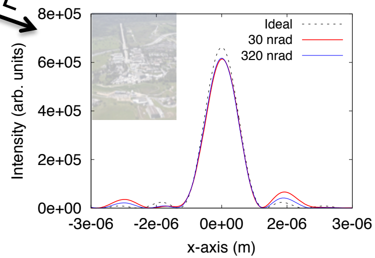
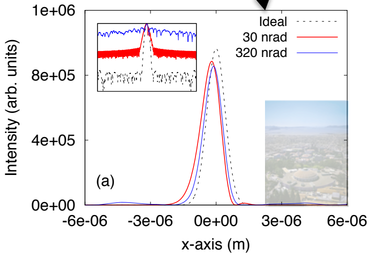


W > L



W < L



System coherence length (W)

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Angular radius ($1/e^2$)

In a diffraction-limited optic, W > L (Mirror length)

Effect of slope errors on the performance of mirrors for x-ray free electron laser applications

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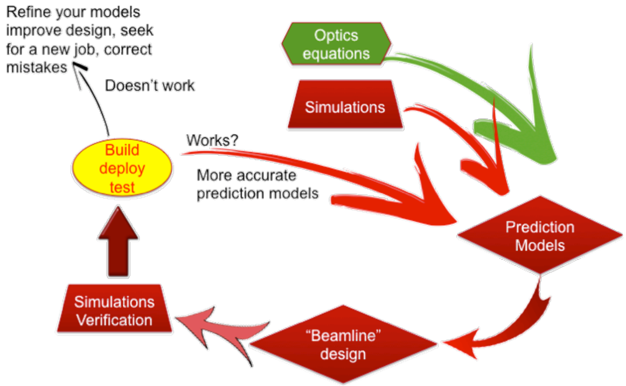
But… be careful! Not knowing the entire validity of the model, can be dangerous!

In a diffraction-limited optic, with W> L (classical FEL cases), only shape errors are important and slope errors, in principle, does not play any role in spot enlargement or beam inhomogeneity

Therefore…

Exercise:
Estimate and simulate, if needed, the spot size of this beamline and the required mirror specifications!



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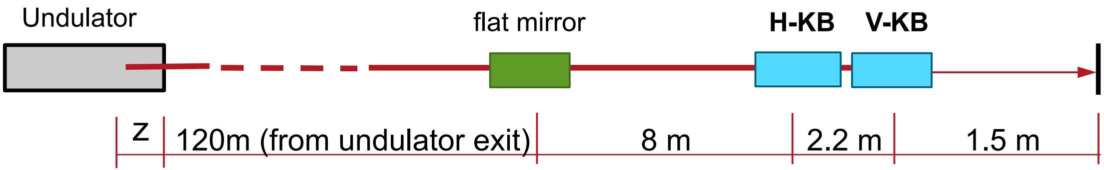
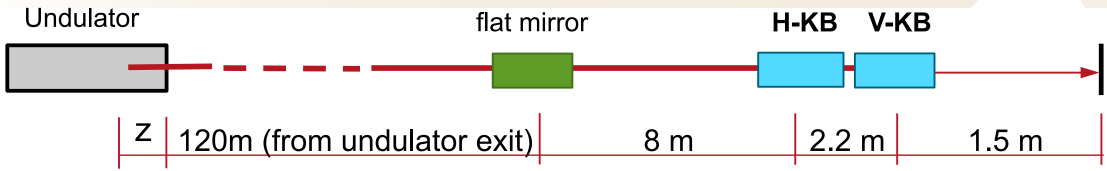
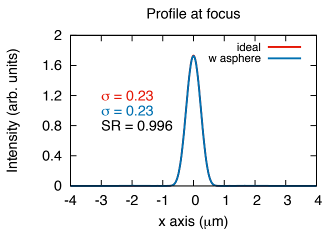


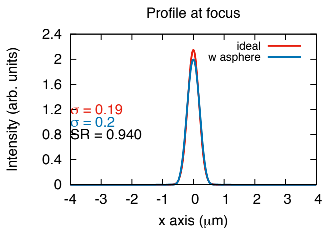
Simulations and models give very similar results
The simulation give the correct result.
Is the question that is wrong!

Not an easy answer – Example: diffraction limited spot





500 eV



1300 eV

$$S_{FWHM} = \frac{\lambda}{2 L \sin\vartheta / r'}$$

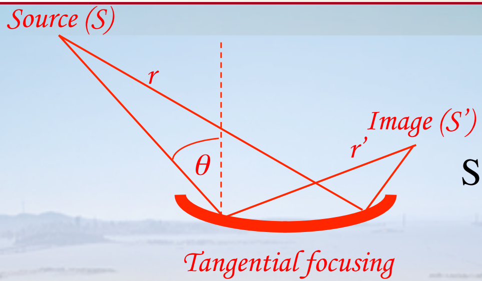
Not the mirror length but the beam footprint

Simulated FWHM 0.54	Simulated FWHM 0.45
Calculated FWHM 0.54	Calculated FWHM 0.48

Simulation and model in good agreement

And, if r' is short, be sure to use the proper f-number

How to treat mirror defects



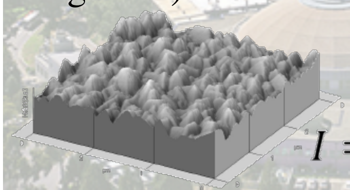
S'= (r'/r) S

Adding rms slope errors σ_{SE}

$\Delta s' = 2\, r' \sigma_{SE}$

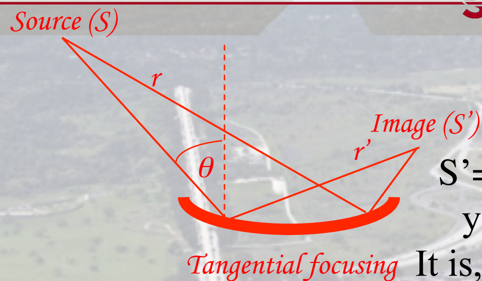
$S' = \sqrt{((r'/r)S)^2 + (2\, r'\sigma_{SE})^2}$

Taking into account the effect of σ_R (rms roughness)



$$I = I_0 e^{-\left(\frac{4\pi\sigma_R \sin\vartheta}{\lambda}\right)^2}$$

Pretty much it works!



S'= (r'/r) S

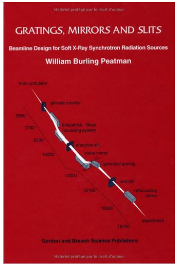
yes but…

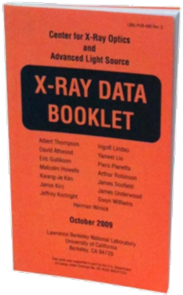
It is, usually, a diffraction limited spot

$$S_{FWHM} = \frac{\lambda}{2\, L \sin\vartheta / r'}$$

Slopes not that important, more to come.....

Make extensive use of formula/models universally accepted



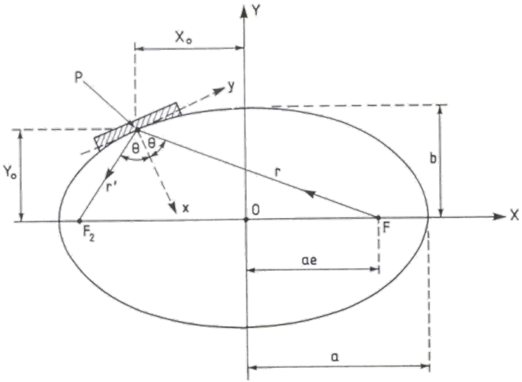


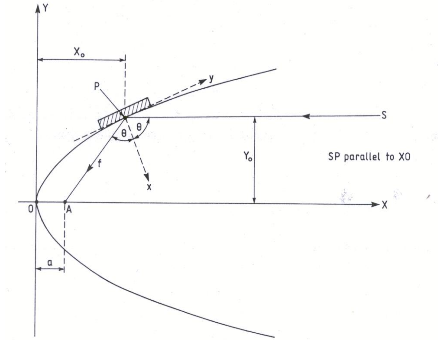
Tangential focus:

$$\left(\frac{1}{r}+\frac{1}{r'_t}\right)\frac{\cos\vartheta}{2}=\frac{1}{R}$$

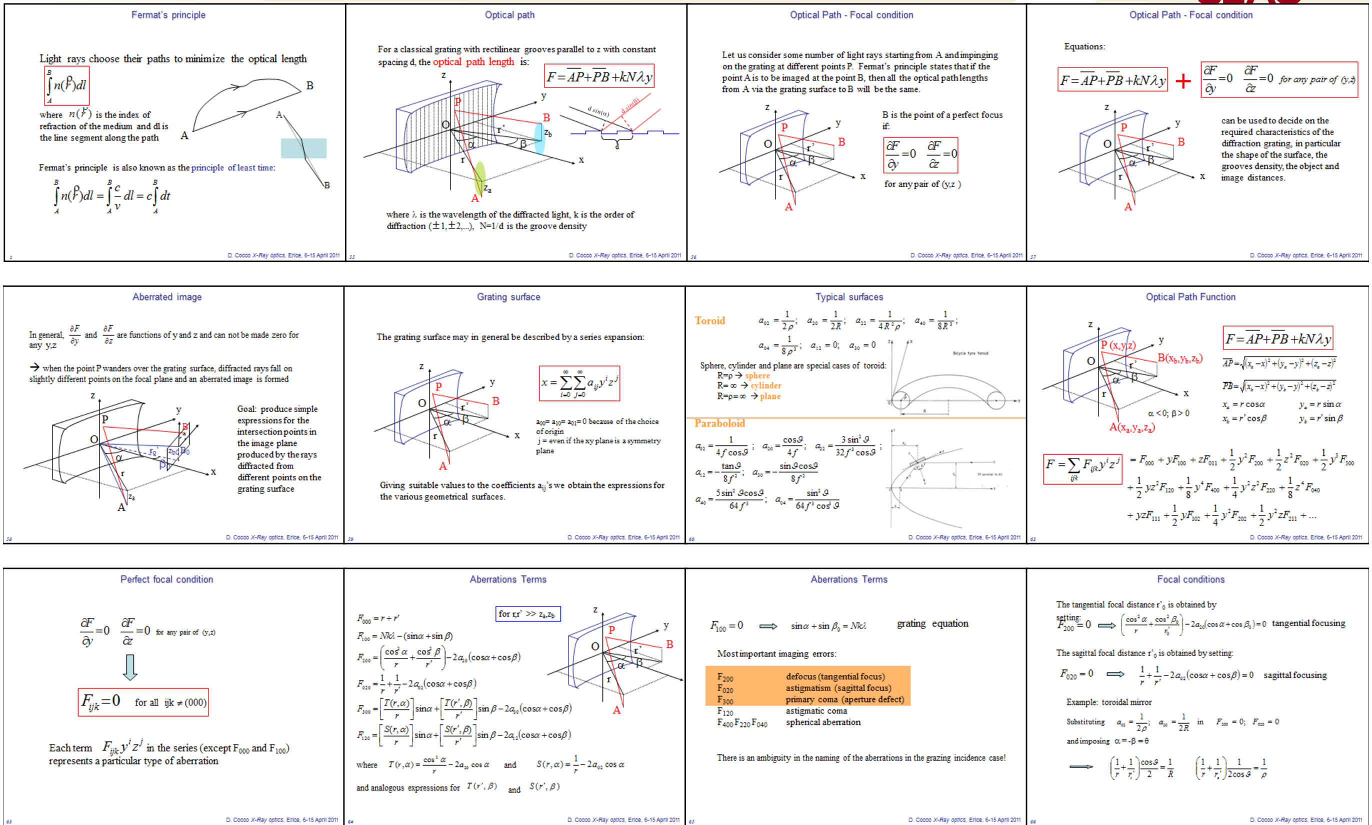
Sagittal focus:

$$\left(\frac{1}{r}+\frac{1}{r'_s}\right)\frac{1}{2\cos\vartheta}=\frac{1}{\rho}$$





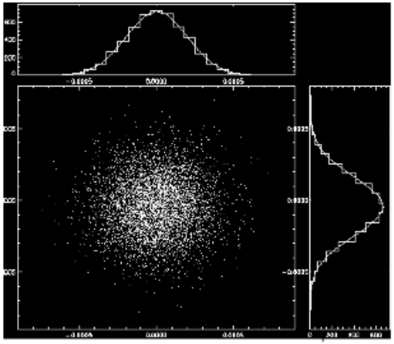
Beamline Design for Synchrotron Radiation

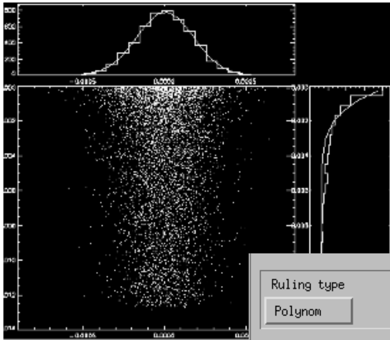


Courtesy of A. Bianco

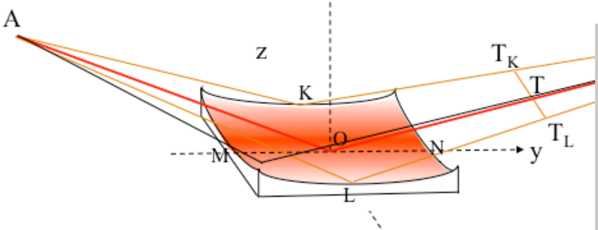
Beamline Design for Synchrotron Radiation

But, as good as you are, you should check it and optimize the design after ray tracing!

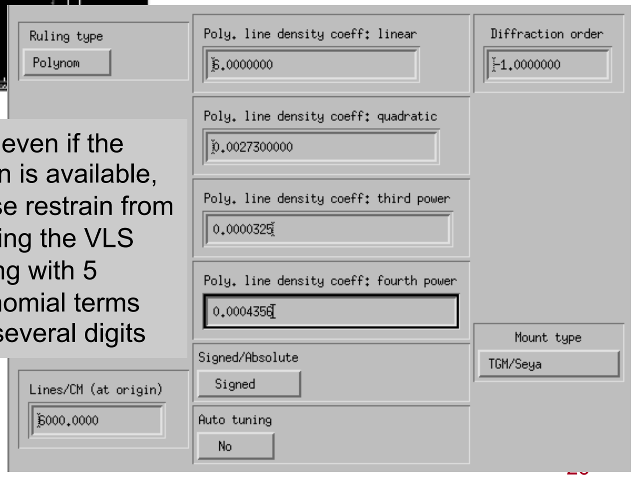




Always double check slope errors, groove density (for VLS gratings), combined effect of different optics, source variation and so on…



And, even if the option is available, please restrain from defining the VLS grating with 5 polynomial terms and several digits



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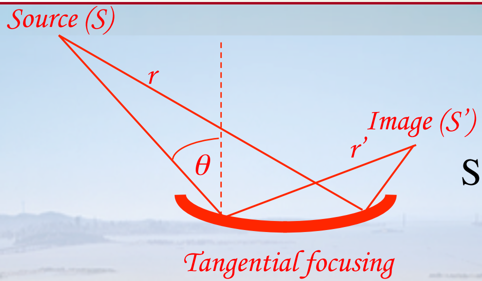

S'= (r'/r) S

Adding rms slope errors σ_{SE}

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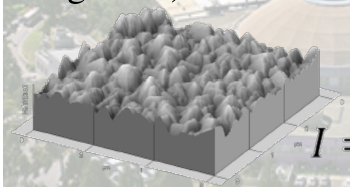

$$I = I_0 e^{-\left(\frac{4\pi\sigma_R \sin\vartheta}{\lambda}\right)^2}$$

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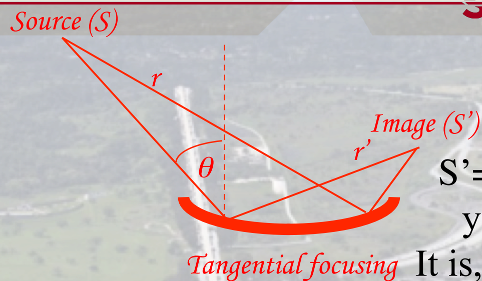

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It is, usually, a diffraction limited spot

$$S_{FWHM} = \frac{\lambda}{2\, L \sin\vartheta / r'}$$

Shape errors effect calculated by using the Strehl Ratio!

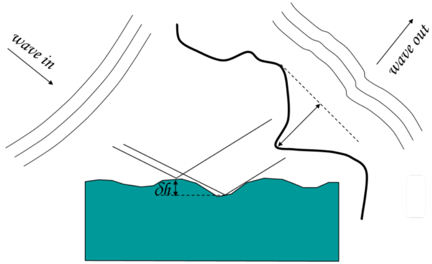
Shape errors effect

$$\text{Strehl Ratio} \approx e^{-(2\pi\varphi)^2} \approx 1-(2\pi\varphi)^2$$

The Strehl Ratio (SR) is defined as a ratio of the maximum intensity in the focus, with and without wave front distortions which are introduced by the optics

$$\varphi = \frac{2\delta h \sin\vartheta}{\lambda}$$

φ is the wave distortion (phase)



$$\delta h = \lambda \frac{\sqrt{1-Strehl\quad Ratio}}{4\pi \sin\vartheta}$$

Maximum acceptable rms shape error for a given Strehl Ratio
SR ≥ 0.8 (according to the Marechal Criterion) is necessary to have "good" optical system

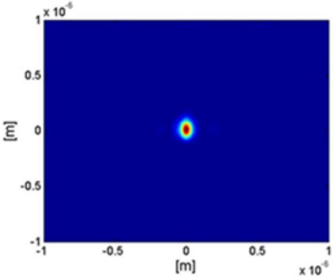
- ϑ → Angle of incidence dependent (larger angles need better shape errors)
- λ → Wavelength depended (shorter wavelengths needs better shape errors)
- δh → This is the value we must "specify" for the mirrors

For a 12 mrad incidence mirror system and 3 mirrors, the required shape errors are:

1.6 nm rms @ 1.3 keV
4.2 nm rms @ 0.5 keV

Shape errors effect

The Marechal Criterion states that a good optical system has a SR ≥ 0.8; e.g.
In focus: the *Gaussian* spot intensity is ≥ 0.8 of the unperturbed *Gaussian* spot intensity



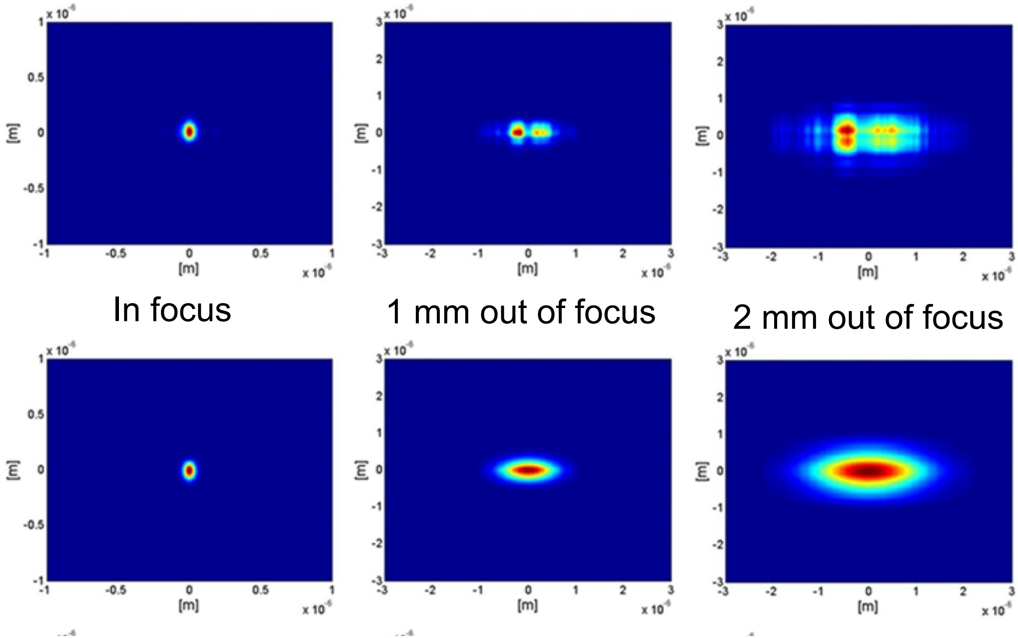
In focus

Yes… but what if working out of focus:

+Simulations of 3 mirrors in one direction and 1 in the other for a global SR of 0.8

Shape errors effect – simulation supported decision!

We need better………..



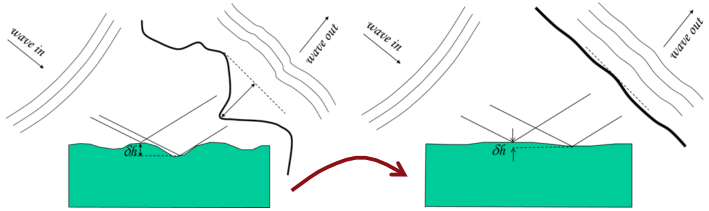
SR≈0.8+

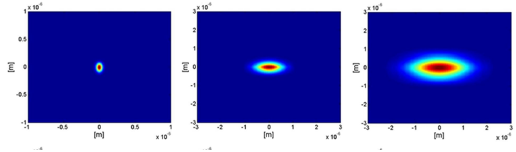
SR≈0.97*

+Simulations of 3 mirrors in one direction and 1 in the other for a global SR of 0.8

* Simulation made with state of the art CXI mirrors

LCLS beamlines upgrade





SR ≥ 0.80
if in focus only

SR ≥ 0.97

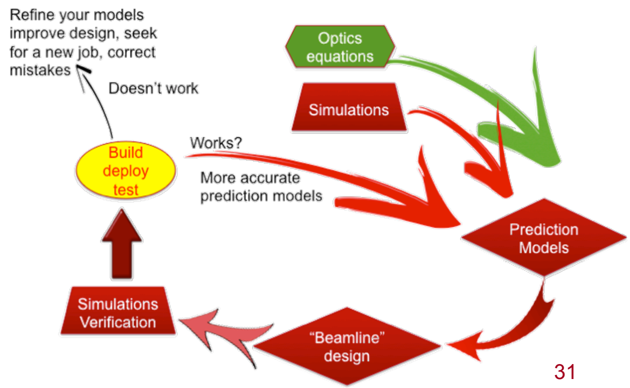
$$\text{Strehl Ratio} \approx e^{-(2\pi\varphi)^2} \approx 1-(2\pi\varphi)^2$$

$$\varphi = \frac{2\delta h \sin\vartheta}{\lambda}$$

$$\delta h = \lambda \frac{\sqrt{1-Strehl \quad Ratio}}{4\pi \sin\vartheta}$$

HXR; 1.35 mrad, 13 keV → **0.56 nm rms**

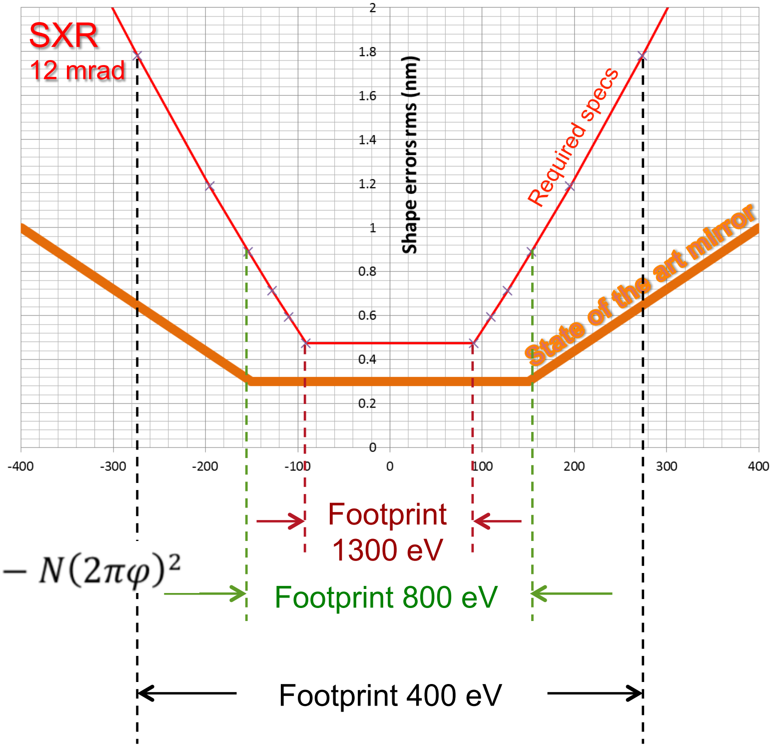
SXR; 12.0 mrad, 1.3 keV → **0.6 nm rms**



LCLS beamlines upgrade

$$SR \approx e^{-(2\pi\varphi)^2} \Rightarrow \varphi = \frac{2\delta h \sin\vartheta}{\lambda}$$

$$\delta h = \lambda \frac{\sqrt{1 - Strehl\ \ Ratio}}{4\pi \sin\vartheta}$$



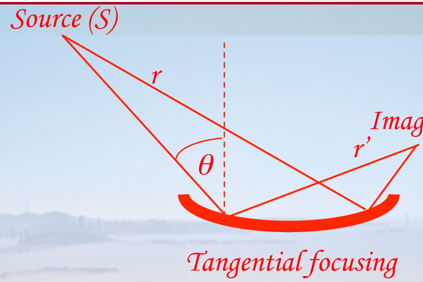
With more than one mirror:

$$SR = e^{-(2\pi\varphi_1)^2} \cdot e^{-(2\pi\varphi_2)^2} \ldots \approx 1 - N(2\pi\varphi)^2$$

$$\delta h = \lambda \frac{\sqrt{1 - Strehl\ \ Ratio}}{4\pi \sin\vartheta \sqrt{N}}$$

How to treat mirror defects

SLAC



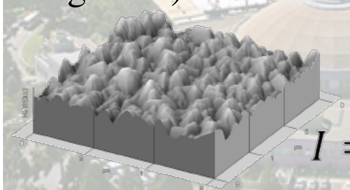
S'= (r'/r) S

Adding rms slope errors σ_{SE}

$\Delta s' = 2\, r' \sigma_{SE}$

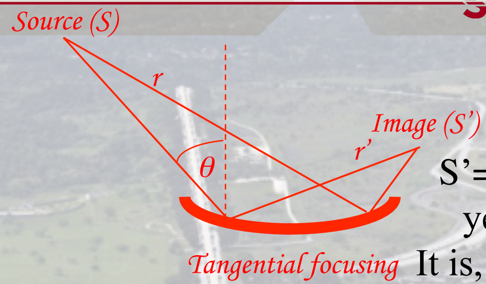
$S' = \sqrt{((r'/r)S)^2 + (2\, r'\sigma_{SE})^2}$

Taking into account the effect of σ_R (rms roughness)



$$I = I_0 e^{-\left(\frac{4\pi\sigma_R \sin\vartheta}{\lambda}\right)^2}$$

Pretty much it works!



S'= (r'/r) S

yes but…

It is, usually, a diffraction limited spot

$$S_{FWHM} = \frac{\lambda}{2\, L \sin\vartheta / r'}$$

Adding rms SHAPE errors δh

One can calculate the phase error

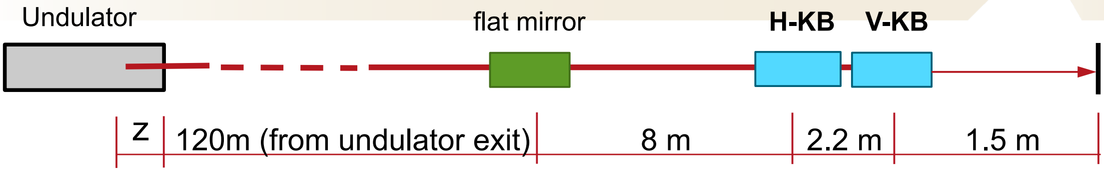
$$\varphi = \frac{2\delta h \sin\vartheta}{\lambda}$$

and the Strehl Ratio:

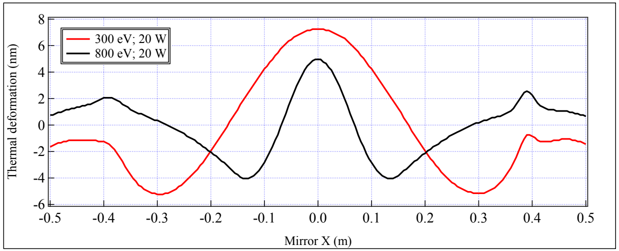
$$SR \approx e^{-(2\pi\phi)^2} \approx 1-(2\pi\phi)^2$$

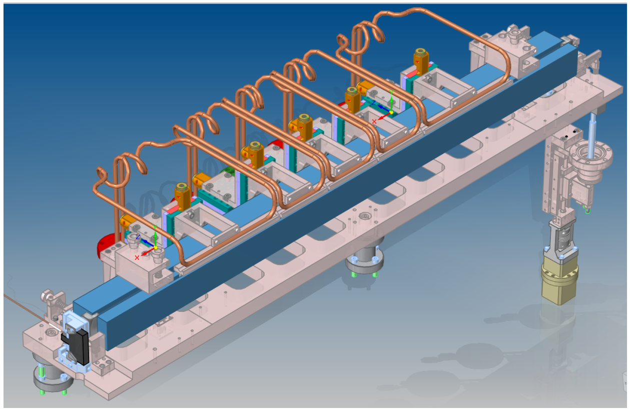
Be careful on asking for the correct SR

Adding further effects



What if now one introduces the thermal bump and mechanical distortions?

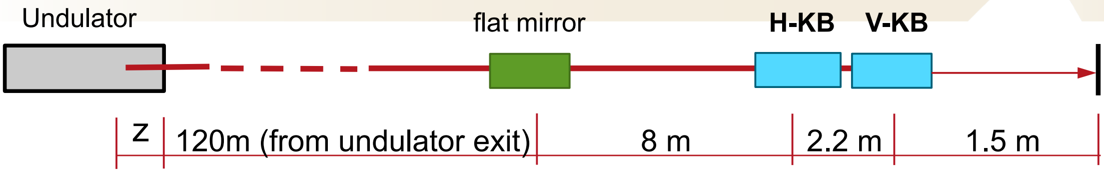




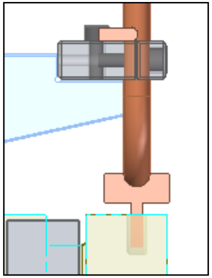
Process: Optimizing the Cooling and holder/bender design to minimize the wavefront distortion

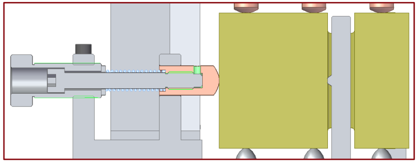
Idea: embed the shape error effect into the FEA optimization process.
Cool, but: how can we really estimate the effect of this "strange" shape errors?
Is 0.5 nm rms a good target? Is too tight? Is too relaxed? And, on which footprint do we have to calculate?

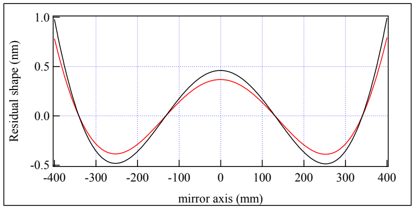
Adding further effects



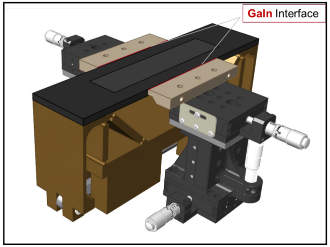
What if now one introduces the thermal bump and mechanical distortions?

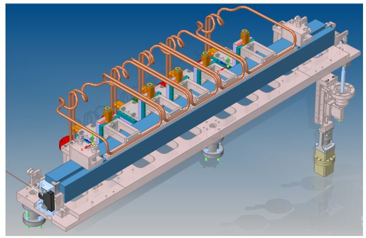






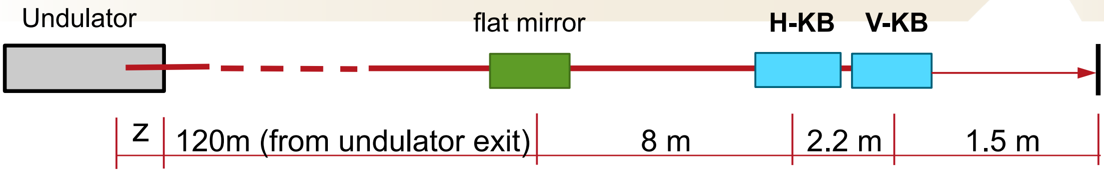
Cooling optimizations, effect of GaIn on the benders, mechanical induced distortions… One can't just minimize everything.





Idea: embed the shape error effect into the FEA optimization process.
Cool, but: how can we really estimate the effect of this "strange" shape errors?
Is 0.5 nm rms a good target? Is too tight? Is too relaxed? And, on which footprint do we have to calculate?

Adding further effects – model validation



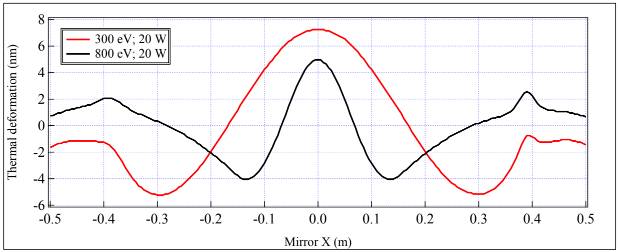
Photon energy (eV)	Max power with SR ≥ 0.97	Max power with SR ≥ 0.8	SR with 200 W incident
200	43 W	112 W	0.36
600	83 W	> 200 W	0.82
900	114 W	> 200 W	0.90
1300	42 W	109 W	0.32

$$SR^* = e^{-(2\pi\varphi_1)^2} \cdot e^{-(2\pi\varphi_2)^2} \ldots$$

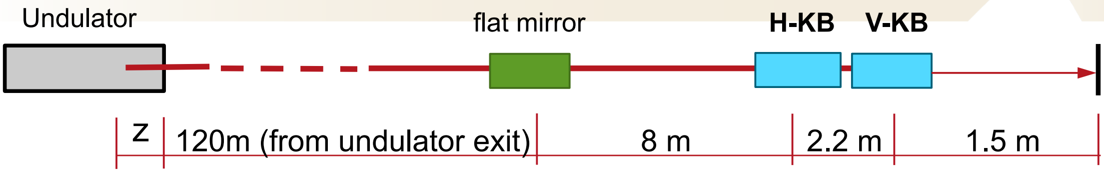
$$\varphi = \frac{2\delta h \sin\vartheta}{\lambda}$$

* Known to work only for SR close to 1

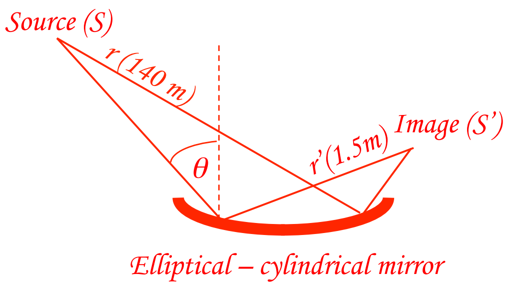
We have started our optimization by calculating the rms shape errors over 2 FWHM and used that to compute the SR.

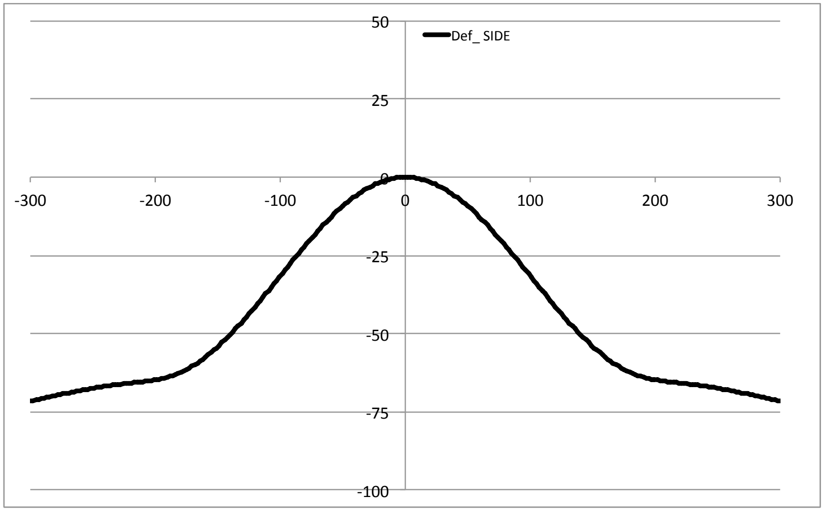


How to calculate this effect?

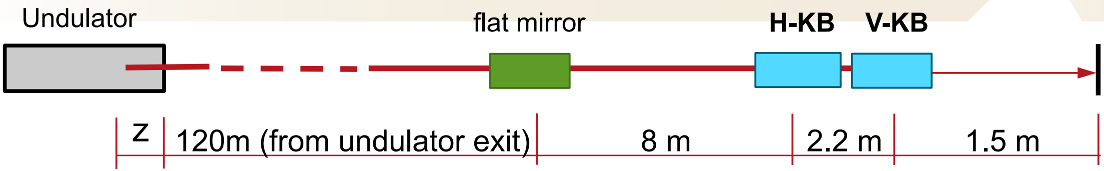


500 eV, including thermal deformations with 200 W incident;
Simple case: 1D, 1 elliptical mirror





How to calculate this effect?



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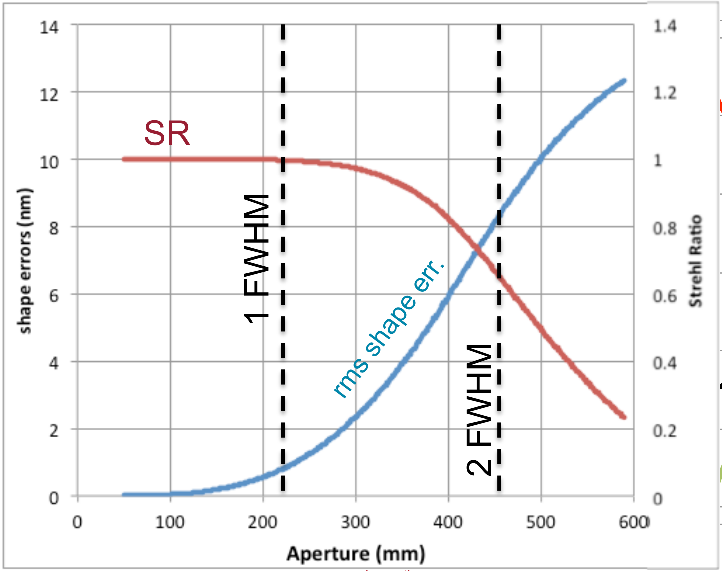
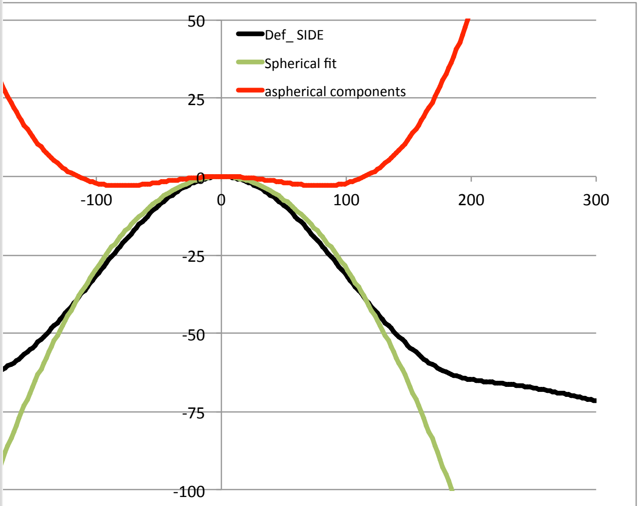
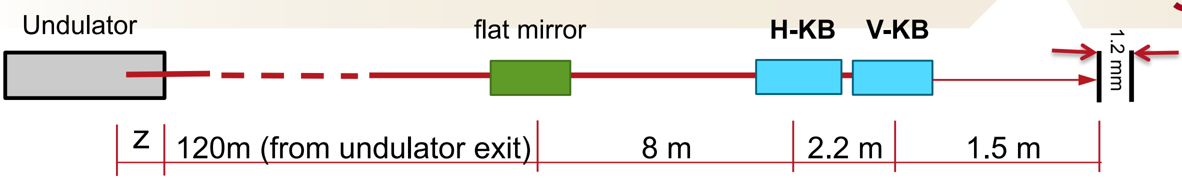
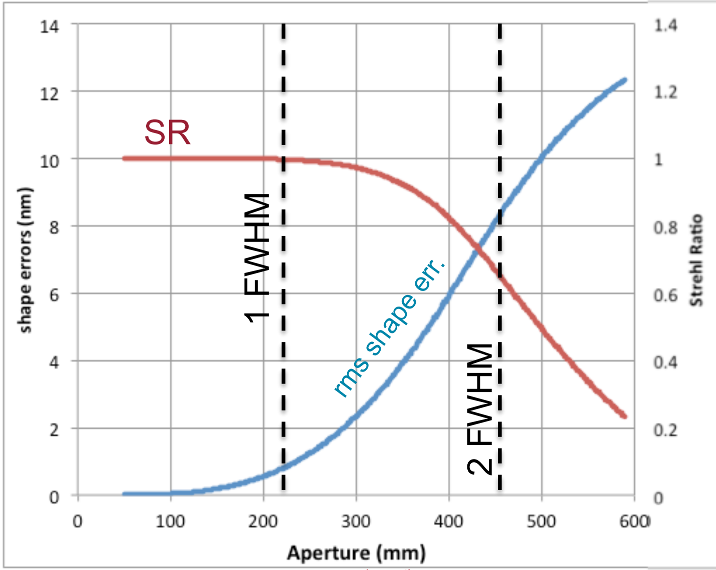


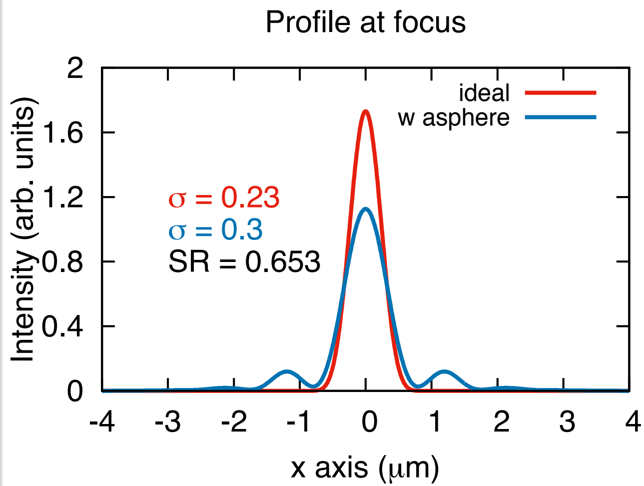


How to calculate this effect?

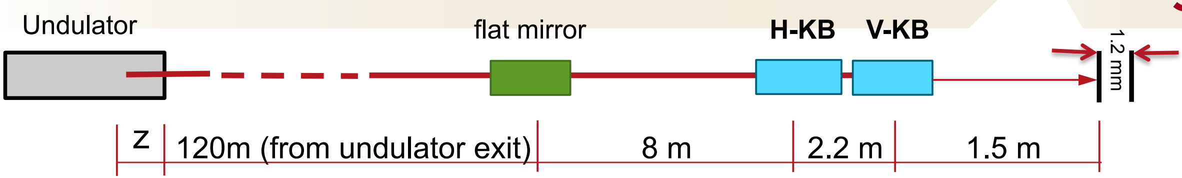


500 eV, including thermal deformations with 200 W incident;
Simple case: 1D, 1 elliptical mirror

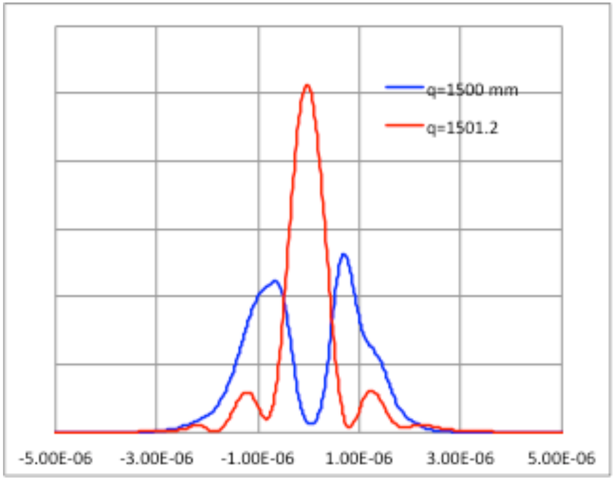


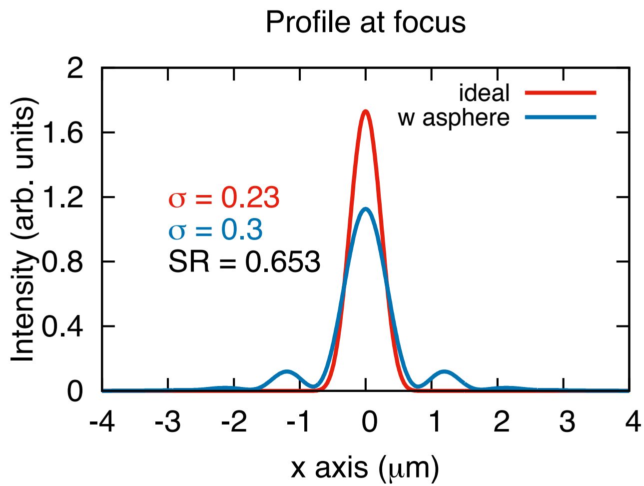


How to calculate this effect?

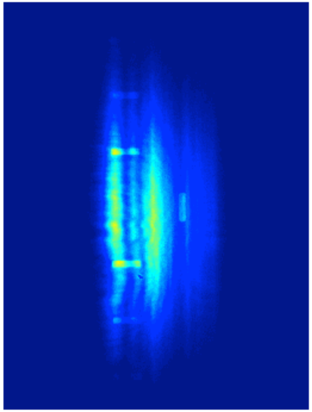


500 eV, including thermal deformations with 200 W incident;
Simple case: 1D, 1 elliptical mirror



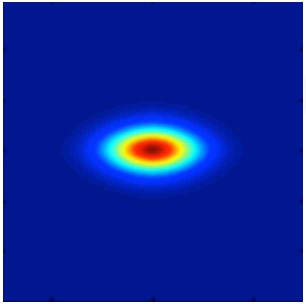


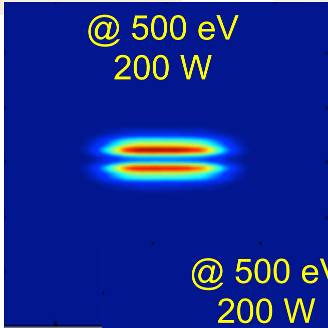
Out of focus effects

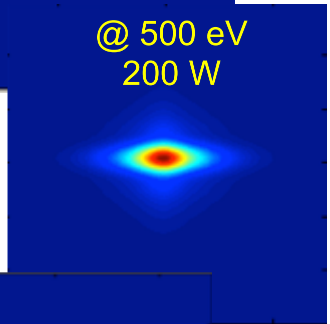


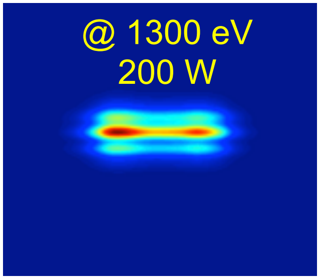
Current limit
shape errors

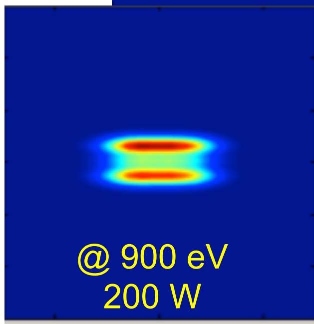
Expected with state
of the art mirrors





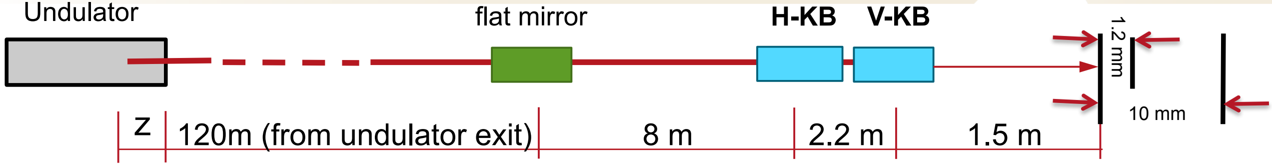




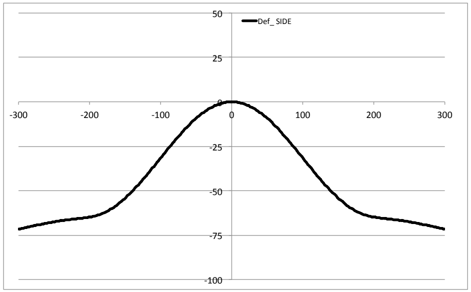


Thermal load will be the next limit. Better know in advance and be ready for that!

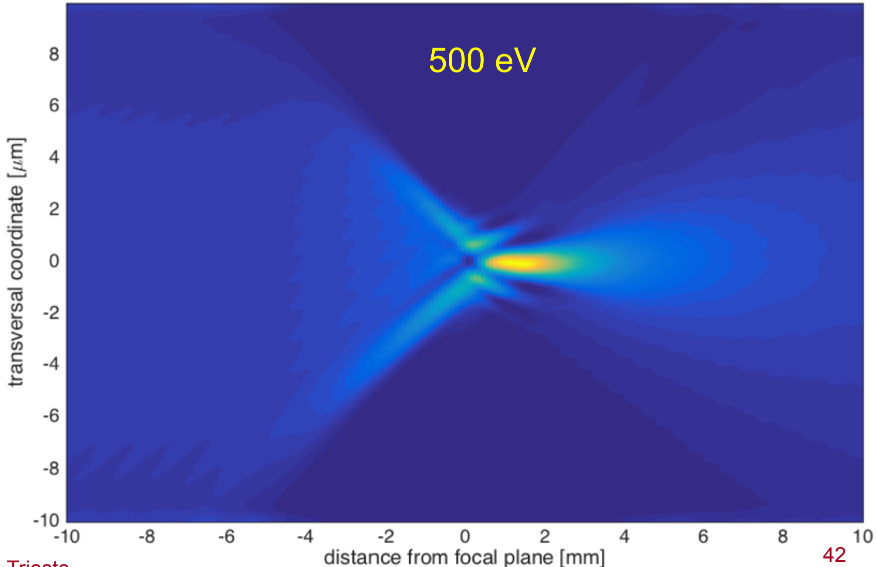
Optimization of KB mirrors



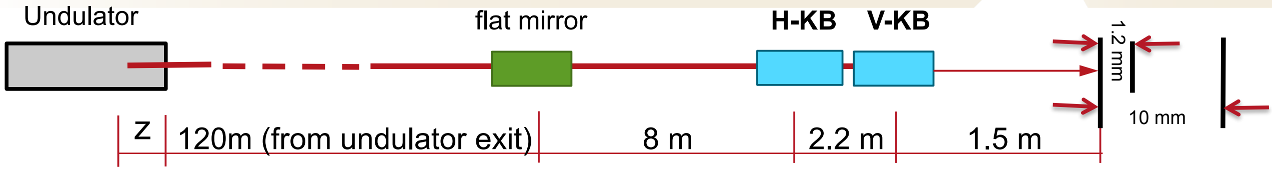
500 eV, including thermal deformations
1 elliptical mirror



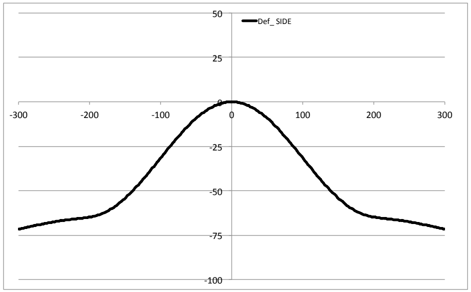
Side cooling



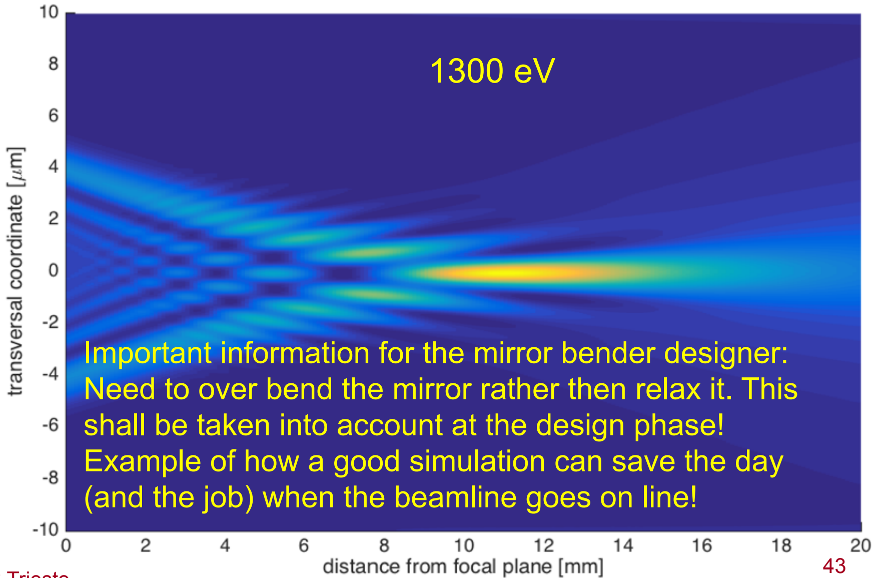
Optimization of KB mirrors



1300 eV, including thermal deformations
1 elliptical mirror

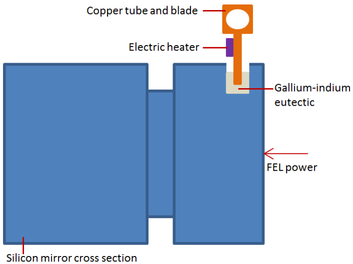


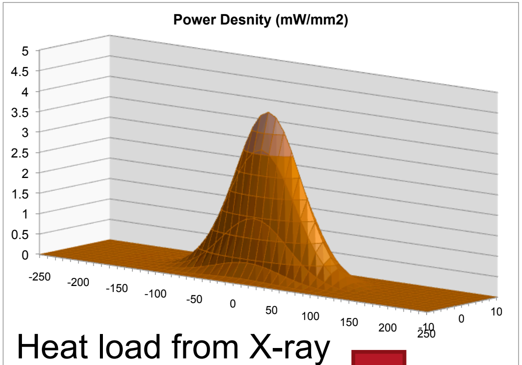
Side cooling

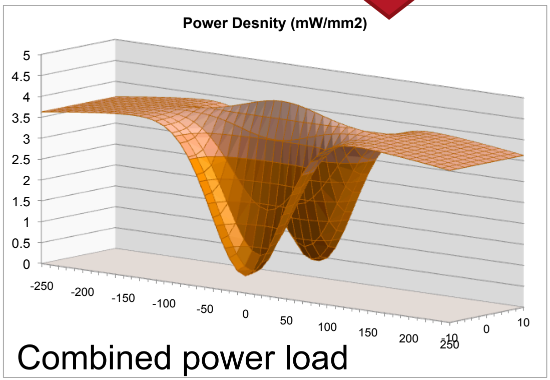


REAL (Resistive Element Adjustable Length) Cooled Optics

To face the incertitude and be ready for LCLS II, we developed a new cooling system to improve the performance at 200 W (project funded by DOE/BES). The decision and the optimization has been made by comparing the FEA with some 2D simulations. Work in progress!

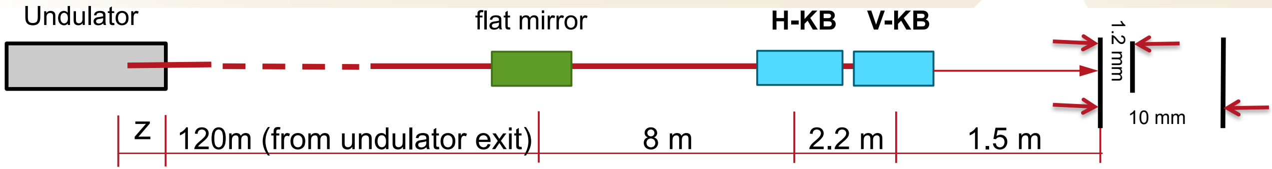




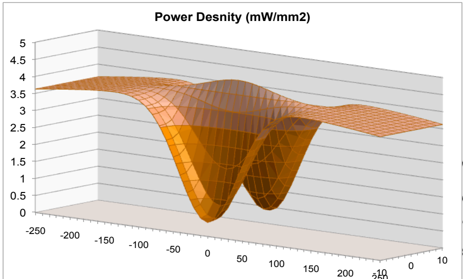


A model to treat the thermal bump and the mechanical deformation, in terms of beamline performance, has been developed and will be, hopefully, published soon.

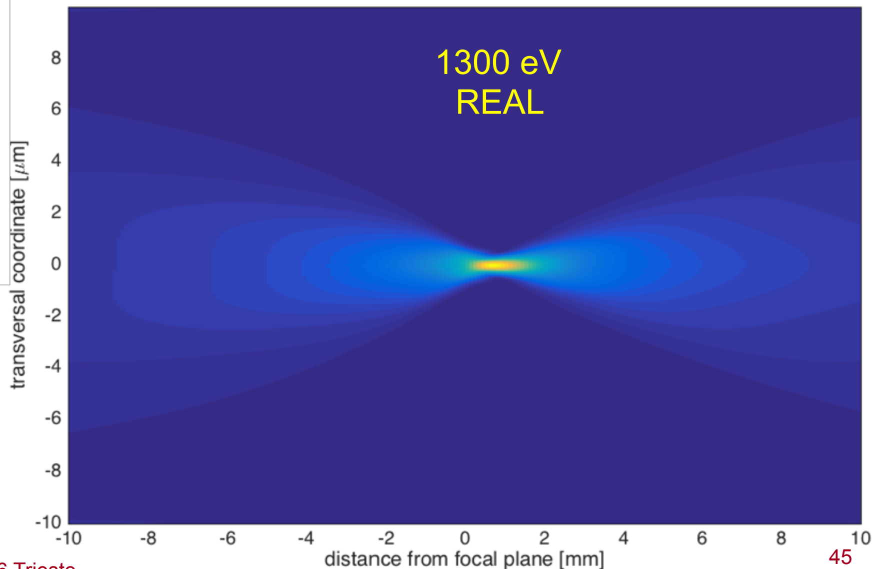
Expected performance with REAL



1300 eV, including thermal deformations
1 elliptical mirror - REAL



Combined power load



REAL is definitively better!

What you (or I) would like to have from simulations

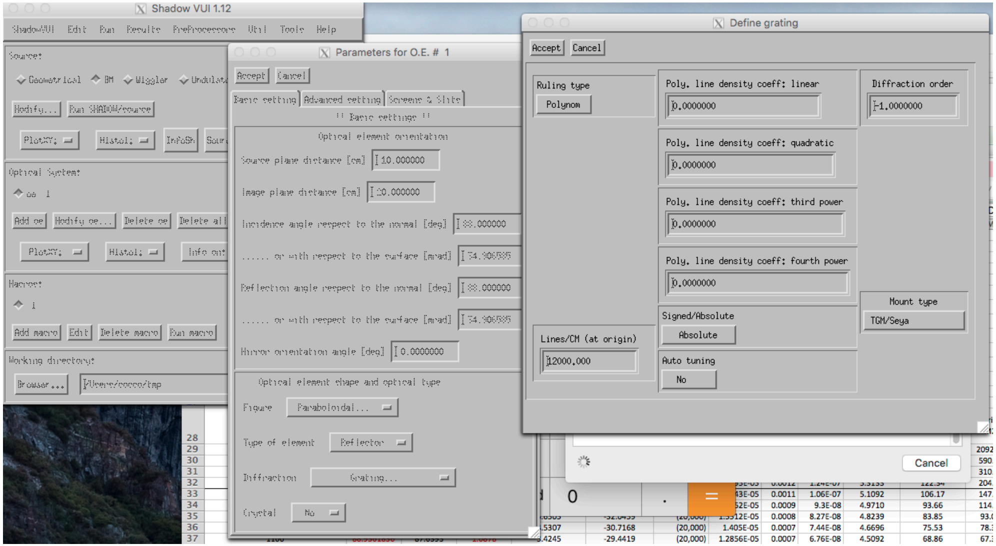
Optical designers are, usually, “engineering physicist”
They handle metrology instrumentations, flexures, FEA, thermal problems, redundant meetings, mechanical complexity, installations programs… they need simple systems

expecially if they lives in nice places
FYI we have open positions in California, at both SLAC (ref. D. Cocco) and Berkeley (ref. K. Goldberg) (BTW the latter one is on wavefront propagation)

What you (or I) would like to have from simulations

Optical designers are, usually, “engineering physicist”
They handle metrology instrumentations, flexures, FEA, thermal problems, redundant meetings, mechanical complexity, installations programs…
Simple, and easy to use, softwares are necessary!

This is good (SHADOW)



What you (or I) would like to have from simulations

Optical designers are, usually, “engineering physicist”
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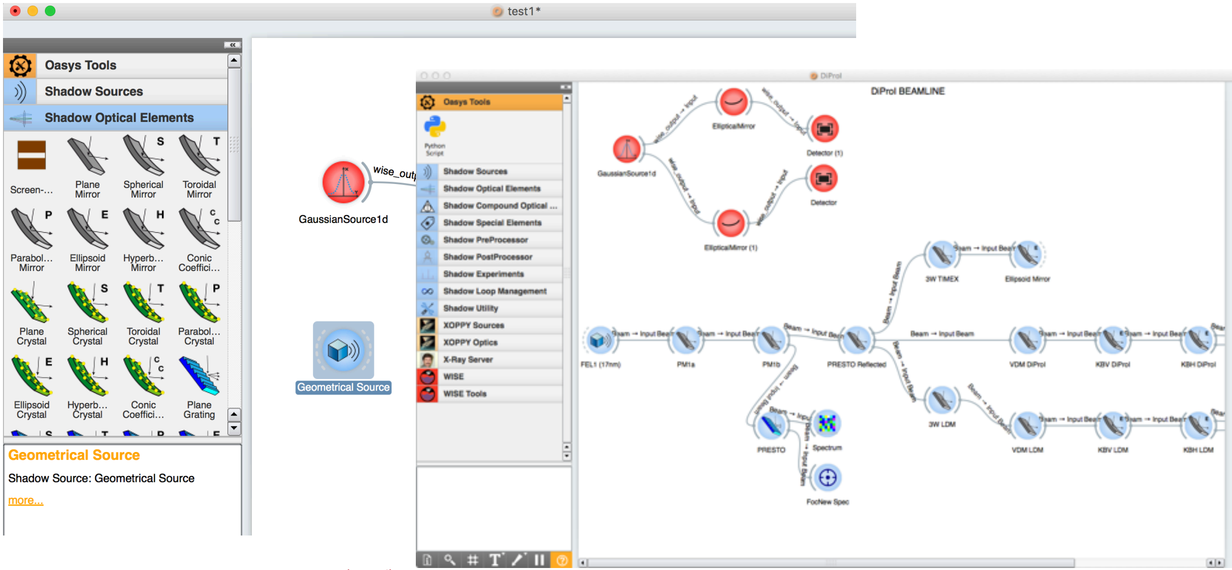
Simple, and easy to use, softwares are necessary!

This is (probably, not yet familiar with it) even better!



What you (or I) would like to have from simulations

Optical designers are, usually, "engineering physicist"
They handle metrology instrumentations, flexures, FEA, thermal problems, redundant meetings, mechanical complexity, installations programs…
Simple and easy to use softwares are necessary!

This is not!

```
import wpg.optical_elements
from wpg import Beamline
from wpg.optical_elements import Empty, Use_PP
from wpg.optical_elements import Drift, Aperture
from wpg.optical_elements import Lens,Mirror_elliptical,WF_dist,calculateOPD
bl.append(Aperture(shape='r',ap_or_ob='a',Dx=lengthOM*thetaOM,Dy=range_xy),
          Use_PP(zoom=1., sampling_h=1./0.5, sampling_v=1.,semi_analytical_treatment=0))
bl.append(Mirror_elliptical(orient='x',p=z_M2, q=q_M2,thetaE=thetaOM, theta0=thetaOM,
                            length=lengthOM), Use_PP(semi_analytical_treatment=1))
wf_dist_m2 = WF_dist(1500,100,range_xy,lengthOM*thetaOM, )
calculateOPD(wf_dist_m2, os.path.join(mirror_data_dir,'mirror1.dat'),2,'\t','y',thetaOM, scale=5)
bl.append(wf_dist_m2,Use_PP())
bl.append(Drift(z_M3-z_M2),Use_PP(semi_analytical_treatment=0));
bl.append(Mirror_elliptical(orient='y',p=z_M3, q=q_M3,thetaE=thetaOM, theta0=thetaOM,length=lengthM3),
         Use_PP(semi_analytical_treatment=1))
wf_dist_m3 = WF_dist(100, 1500, range_xy, lengthM3*thetaOM, )
calculateOPD(wf_dist_m3, os.path.join(mirror_data_dir,'mirror2.dat'),2'\t''y',thetaOM, scale=5)
bl.append(wf_dist_m3,Use_PP())
bl.append(Drift(z_focus_M2-z_M3),Use_PP(semi_analytical_treatment=0));
width = 50.e-6     # slit width
dz_blades = 30e-2 # distance between blades
bl.append(Aperture(shape='r',ap_or_ob='o',Dx=50e-3,Dy=50e-3,x= (50e-3/2+width/2),y=0),Use_PP())
bl.append(Drift(dz_blades),Use_PP(semi_analytical_treatment=0));
bl.append(Aperture(shape='r',ap_or_ob='o',Dx=50e-3,Dy=50e-3,x=-(50e-3/2+width/2),y=0),
          Use_PP(zoom_h=0.9,sampling_h=0.9/1.0))
bl.append(Drift(z_M3-z_focus_M2),Use_PP(zoom_h=2.4,sampling_h=2.4/0.4));
bl.append(Aperture(shape='r',ap_or_ob='o',Dx=50e-3,Dy=50e-3,x=0,y=(50e-3/2+width/2)),Use_PP())
bl.append(Drift(dz_blades),Use_PP(semi_analytical_treatment=0))
zz = zz + dz_blades
bl.append(Aperture(shape='r',ap_or_ob='o',Dx=50e-3,Dy=50e-3,x=0,y=-(50e-3/2+width/2)),Use_PP())
bl.append(Drift(z_focus_M2-z_focus_M3-dz_blades),Use_PP(zoom_v=1.4,sampling_v=1.4/0.5))
print bl; bl.propagate(wf)
```

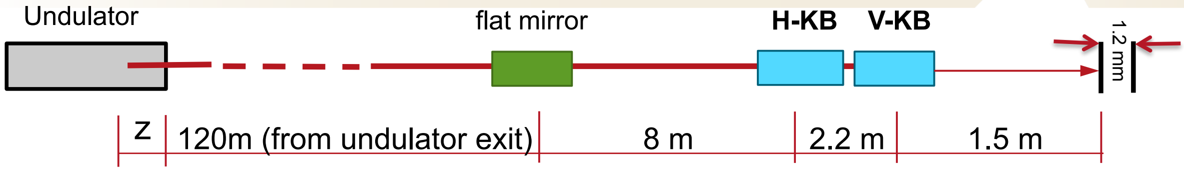
Example of a beamline definition: the SASE3 beamline at the European XFEL will include two horizontal offset mirrors (M1 and M2), a vertical focusing mirror M3, and horizontal and vertical clean-up slits.

What you (or I) would like to have from simulations

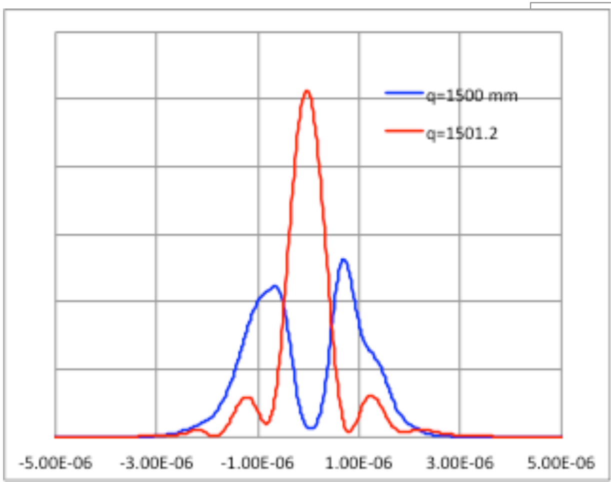
Optical designers are, usually, “engineering physicist”
They handle metrology instrumentations, flexures, FEA, thermal problems, redundant meetings, mechanical complexity, installations programs…
Simple, and easy to use, softwares are necessary!
<u>Being reliable and tested!</u>

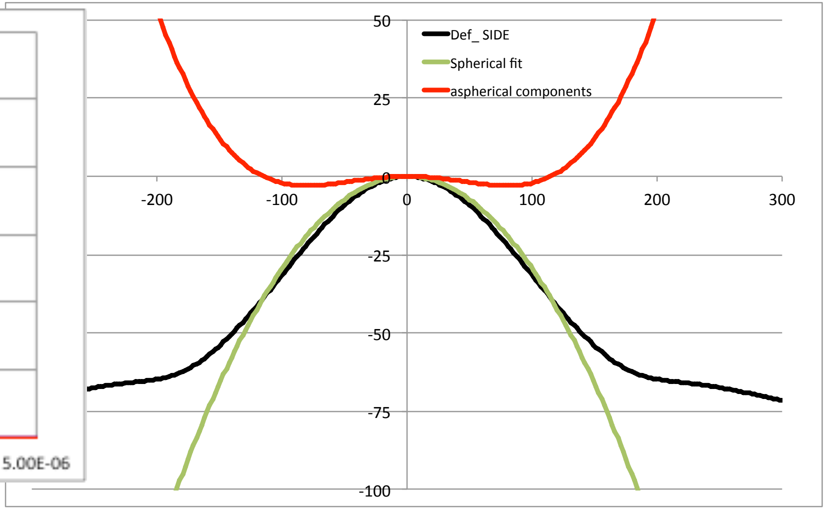
- “Universally” accepted/used wavefront propagation codes (or for fully and partially coherent sources) has yet to come but, a lot of effort is going on:
  - *SRW, WISE, PHASE, HYBRID, WavePropaGator, OASYS…*
  - *X-ray optics simulation using Gaussian superposition technique* ,Mourad Idir, at al, Opt. Express 2011
  - A hybrid method for X-ray optics simulation: combining geometric ray-tracing and wavefront propagation, X. Shi, at al. J. Synch. Rad. 2014
  - J.E. Krist, “PROPER” Optical Modeling and Performance Predictions
  - In house/custom codes ………..

Check validity of simulations (by comparison)



Comparison at 500 eV, including thermal deformations with 200 W incident; Simple case: 1D, 1 elliptical mirror





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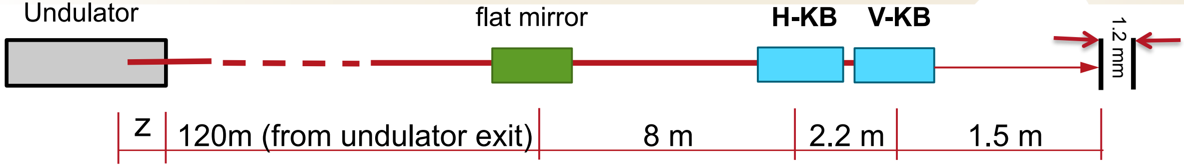
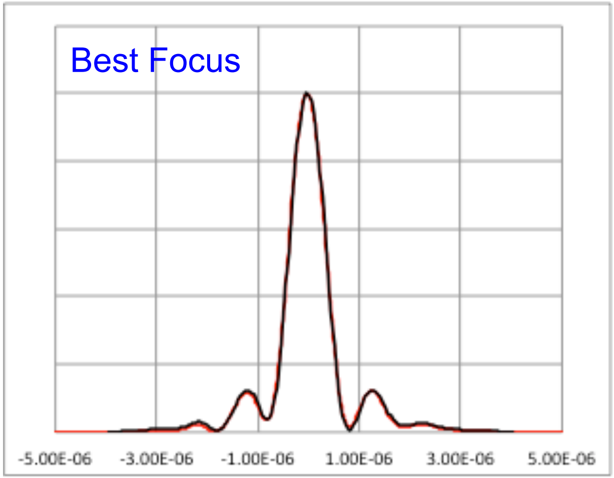
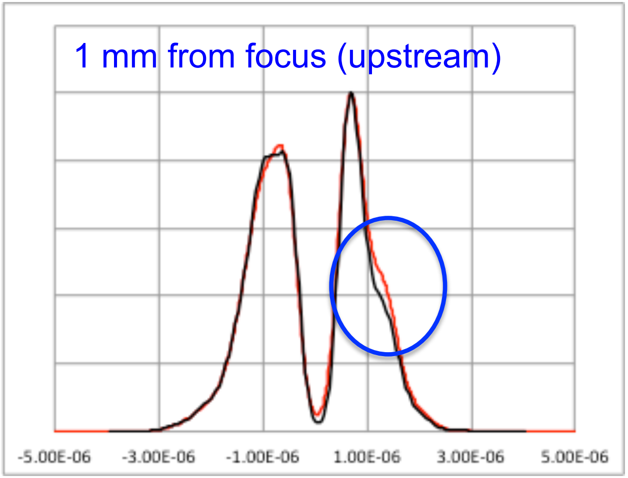


Comparison at 500 eV, including thermal deformations
Simple case: 1D, 1 elliptical mirror

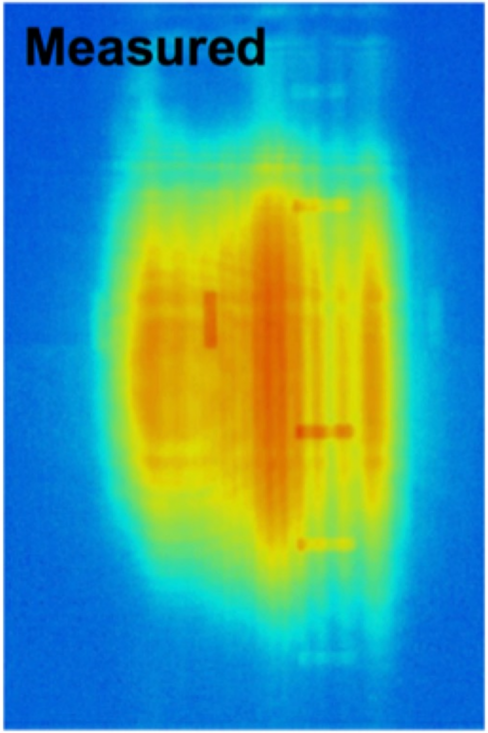




Black: WISE
Red: Kirchhoff Integrals

Check validity of simulations (against measurements)

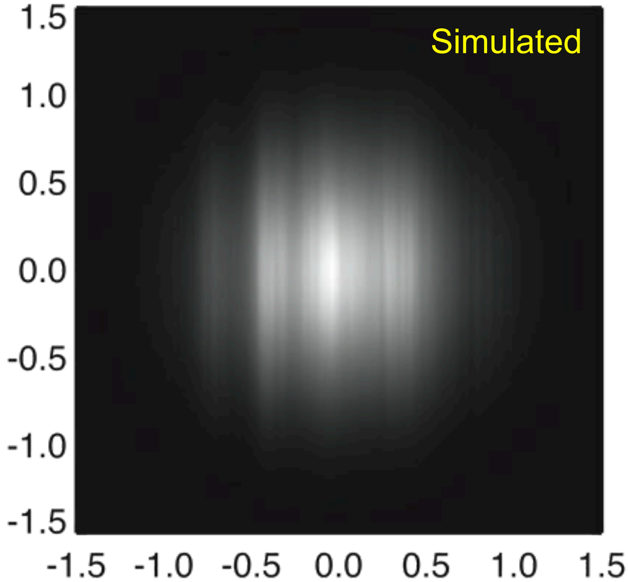
Before (2009)



Predicting the coherent X-ray wavefront focal properties at the Linac Coherent Light Source (LCLS) X-ray free electron laser

Anton Barty[1,2*], Regina Soufli[1], Tom McCarville[1], Sherry L. Baker[1], Michael J. Pivovaroff[1], Peter Stefan[3] and Richard Bionta[1]

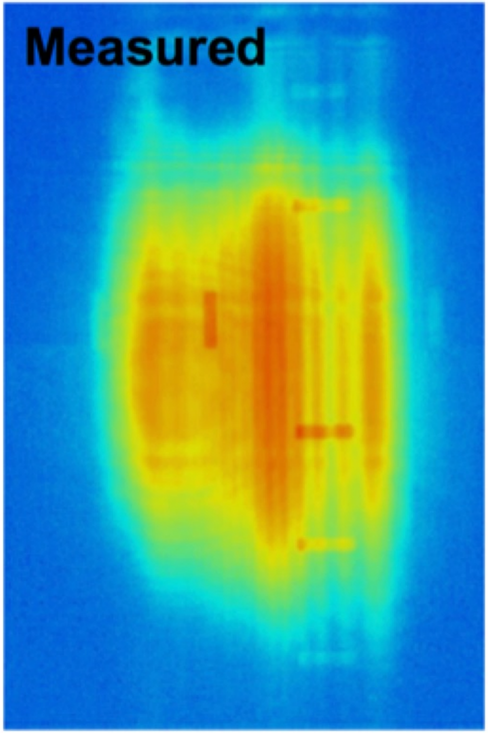
[1] Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore, CA, 94550, USA
[2] Centre for Free Electron Laser Science, Notkestrasse 85, 22607 Hamburg, Germany
[3] SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA
*anton.barty@desy.de

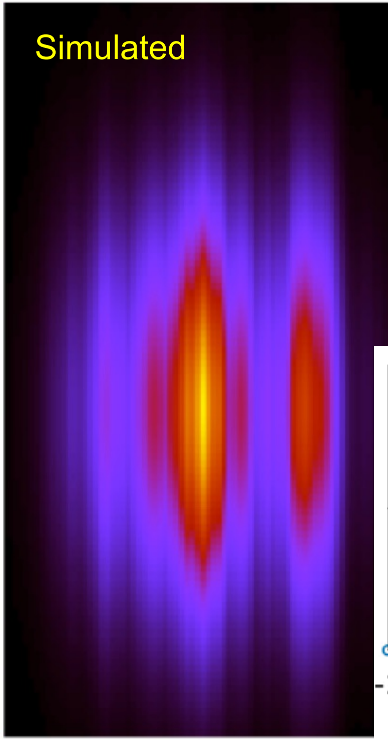


Check validity of simulations (against measurements)

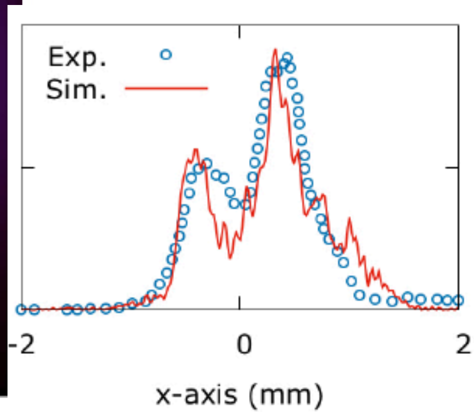
After 2009 (2016)

Submitted to Journal of Synchrotron Radiation





Main difference:
Used measured divergence and longitudinal position of the source



Make simulations more accessible

Optical designers are, usually, "engineering physicist"
They handle metrology instrumentations, flexures, FEA, thermal problems, redundant meetings, mechanical complexity, installations programs…
Simple and easy to use softwares are necessary!
Being reliable and tested!

At the limit you need it!

We need to rely on the result of the simulation at a sufficient level to design and procure the components for the beamline, not to use as a experimental data reference field/intensity distribution normalization.

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Being reliable and tested!

At the limit you need it!

Faster, when needed!

Step 1 Model
Step 2 1D Fourier optics or Kirchhoff integrals
Step 3 2D for nice picture (publication, founding agency, beamline scientists…)

Accepting arbitrary shapes (1D, 2D, high order polynomials) and, why not, remote interfaced with DABAM
Accepting arbitrary source description and, as an option, accepting output from GENESIS….
S2E simulations, including source are not pratical nor useful in most of the cases!

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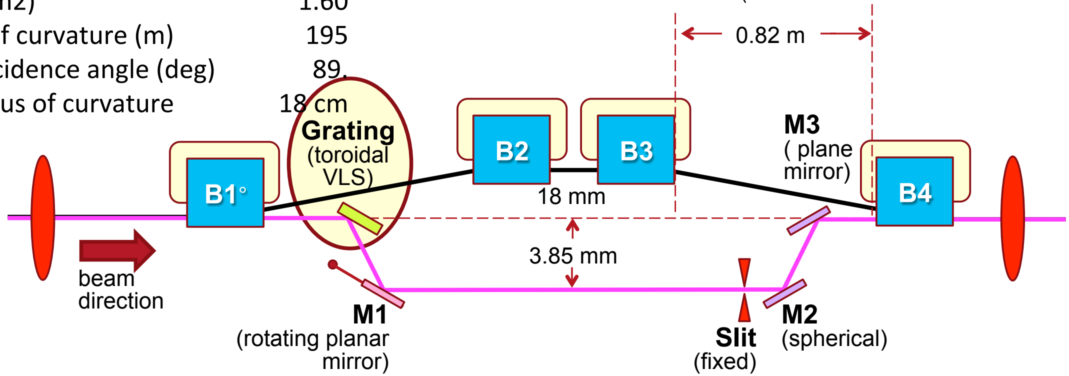
S2E simulations, including source are not pratical nor useful in most of the cases!
…and Hybrid system (e.g. partially coherent) is probably better (if and only if, easy to handle and use!)

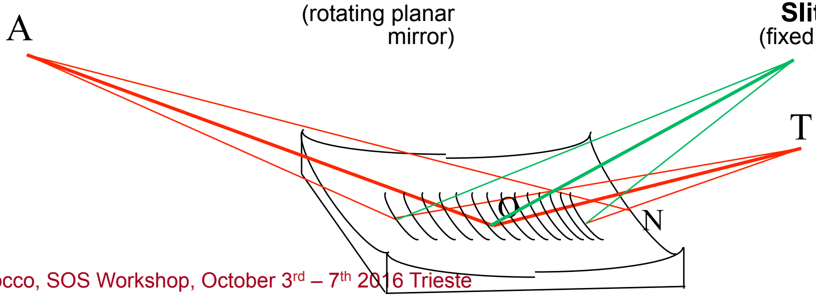
Post mortem simulation – an example

In 2014, the SXR self seeding monochromator for LCLS has been commissioned. It has been entirely designed by using the optical path function (plus diffraction limited contribution) and ray tracing for grating parameter optimization and tolerances

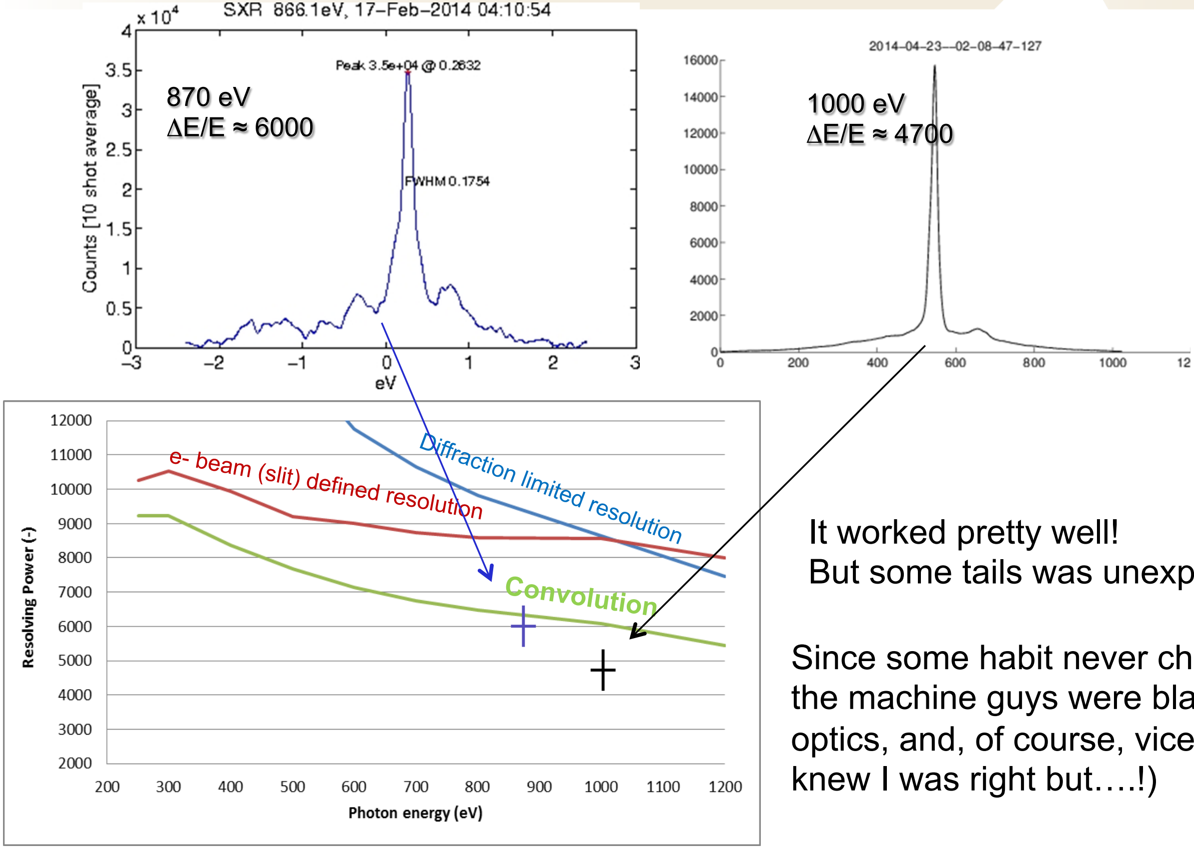
Central groove density (l/mm)	1123
D1 (l/mm2)	1.60
Radius of curvature (m)	195
Fixed incidence angle (deg)	89.
Sag Radius of curvature	18 cm

$$F_{20} = -n\lambda D_1 + \left(\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R} + \frac{\cos^2\beta}{r'} - \frac{\cos\beta}{R} \right)$$





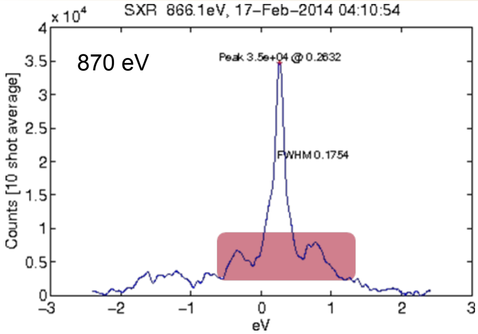
Post mortem simulation – an example

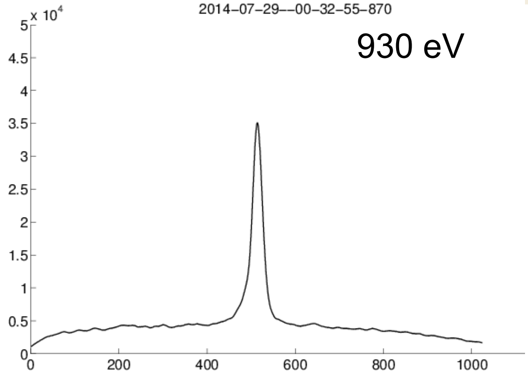


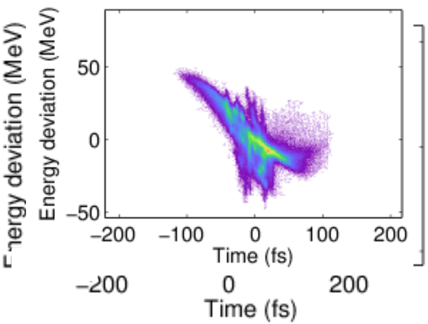
It worked pretty well!
But some tails was unexpected

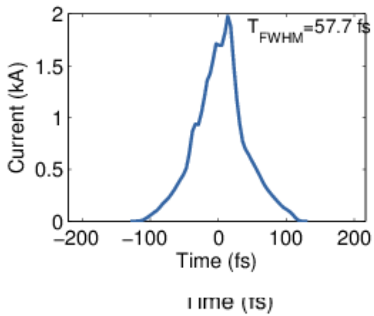
Since some habit never changes, the machine guys were blaming the optics, and, of course, vice versa (I knew I was right but….!)

Post mortem simulation – an example









Post mortem simulation – it's actually good!

Some extensive modeling and simulations has been made after such results

Soft x-ray self-seeding simulation methods and their application for the Linac Coherent Light Source

Svitozar Serkez*
Deutsches Elektronen-Synchrotron (DESY), Hamburg 22607, Germany

Jacek Krzywinski, Yuantao Ding, and Zhirong Huang
SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA
(Received 15 December 2014; published 13 March 2015)

We use the GENESIS code to obtain an electric field distribution in space and time at the end of the SASE undulator. Then we apply a temporal Fourier transform [Eq. (1)] and propagate the transverse distributions for every calculated discrete frequency. Finally, the inverse temporal Fourier transform is performed to go back into space-time domain.

Post mortem simulation – it's actually good!

SLAC

"We found that surface height
errors of installed optics have no significant effect on the
monochromator performance…...

Based on simulations, we found that resolving power of
the monochromator operating without the exit slit varies
from 5400 to 8500, that is close to resolving power with the
3 μm exit slit inserted…..

Simulations with the source position in
the undulator U8 showed a better resolving power than that
the undulator U8 is not active."

Soft x-ray self-seeding simulation methods and their application for the Linac Coherent Light Source

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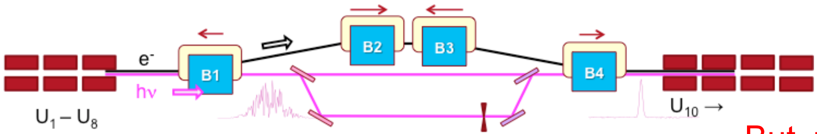
Those results are almost identical to what I obtained with simple models and ray tracing.



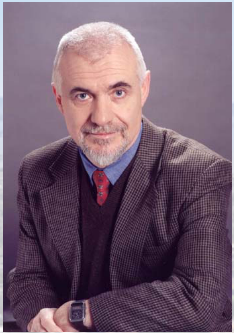
But, this new simulation tools will be very helpful for future Self Seeding design!

If you don't have reasonably user friendly software, you take chances…and rely on proper models or on your good luck!

Conclusions – What it would be nice to have

SLAC

Simulations are like cough syrup. Just because you don't use often or you don't like it, doesn't mean it is not important



Thanks

In memory of
Franco Cerrina (1948-2010)
Pioneer in X-ray optical simulation

User friendly softwares are necessary!

Repository of models to use with coherent or partially coherent source to be updated

Being reliable and tested!
At the limit you need it!
Faster, when needed!

Accepting arbitrary shapes (1D, 2D, high order polynomials) and, why not, remote interfaced with DABAM

Accepting arbitrary source description in an easy way
S2E simulations, including source are not pratical nor useful in most of the cases!

…and Hybrid systems are probably better and more reliable (if easy to handle and use!)

Looking forward to learn a lot from you guys!