Trieste, 04.10.2016

Fast physical optics modelling of x-ray systems

Frank Wyrowski, University of Jena & Wyrowski Photonics UG

Antonie Verhoeven, University of Eastern Finland

Christian Hellmann, Wyrowski Photonics

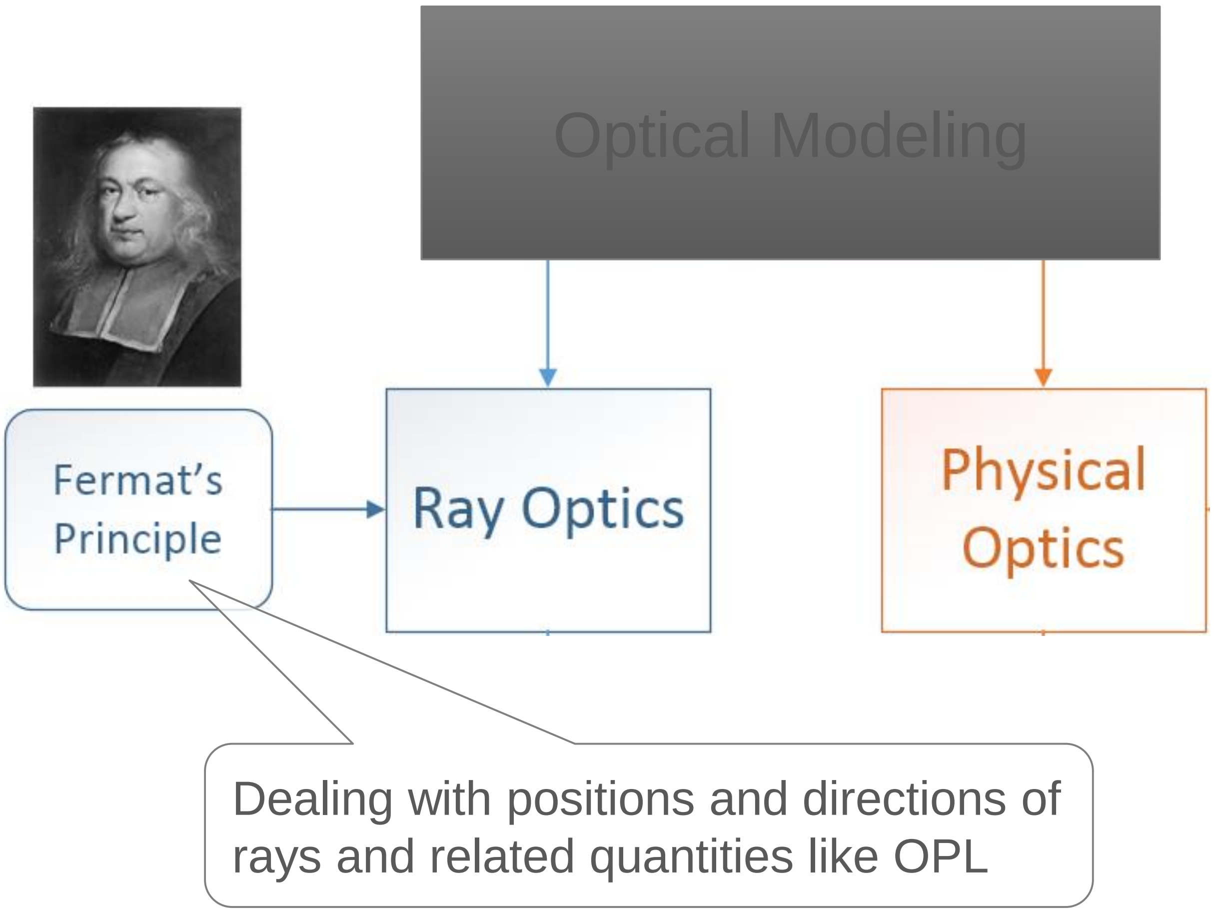
Mourad Idir, BNL

Jena, Germany

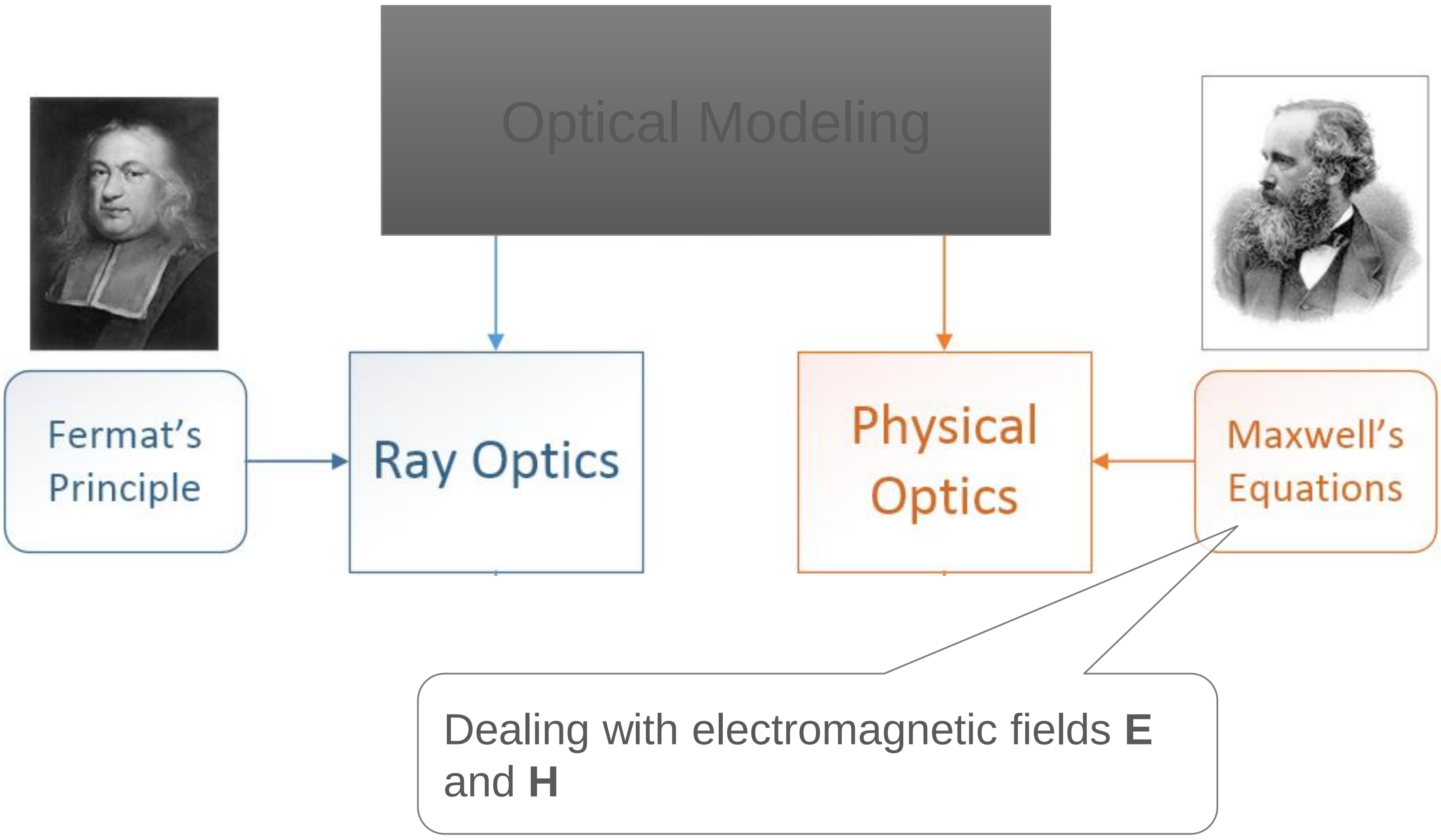
My Three Teams at …

- **Applied Computational Optics Group** at Friedrich Schiller University of Jena
  - R&D in optical modeling and design with emphasis on physical optics.
- **Wyrowski Photonics**
  - Development of fast physical optics software VirtualLab Fusion
- **LightTrans**
  - Distribution of VirtualLab, together with distributors worldwide
  - Service, technical support, seminars, and trainings
  - Optical engineering projects

Ray and Field Tracing



Ray and Field Tracing



Ray and Field Tracing

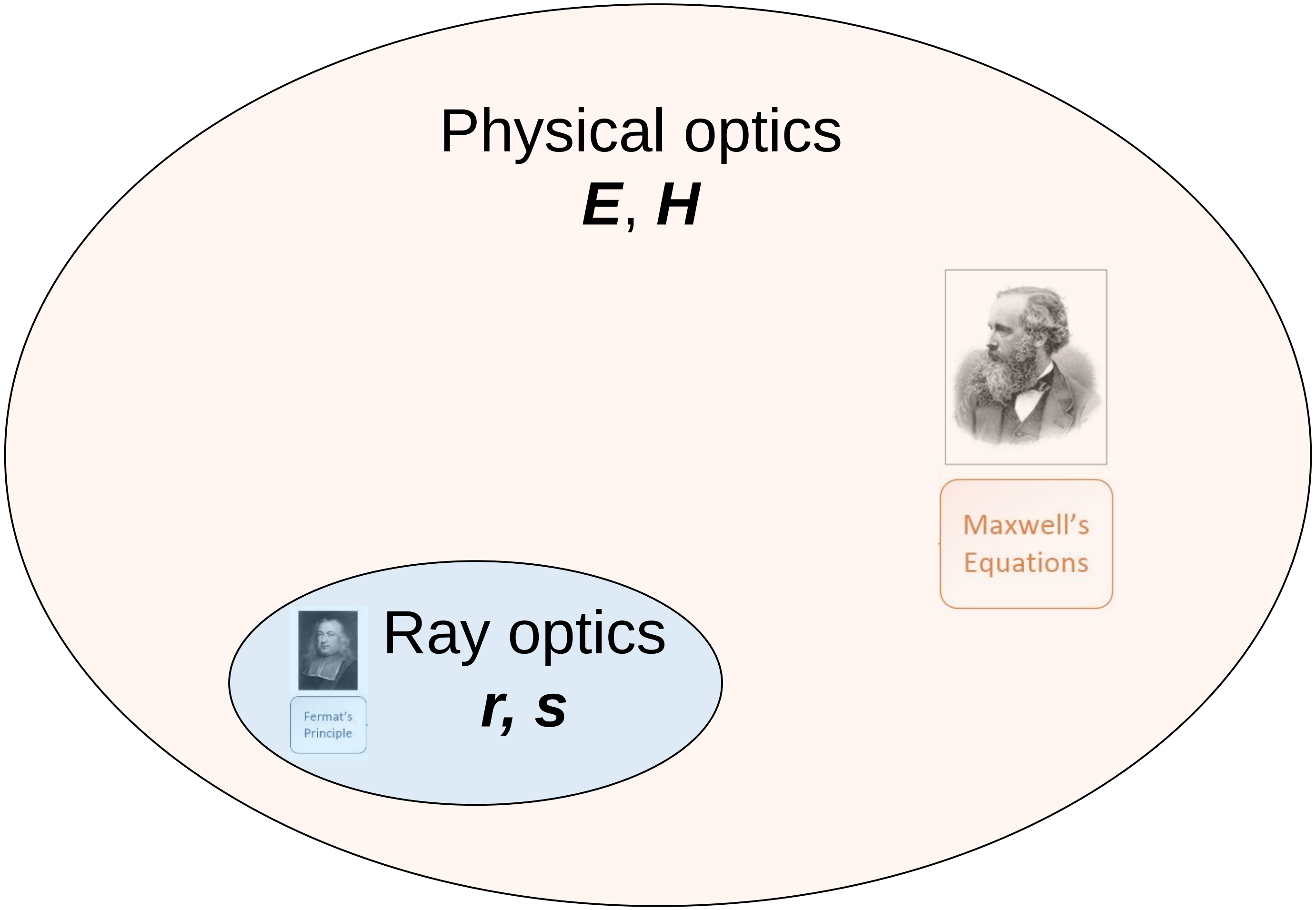
Fermat's Principle

Follows from

Maxwell's Equations

… "forgetting" field information

Ray and Field Tracing



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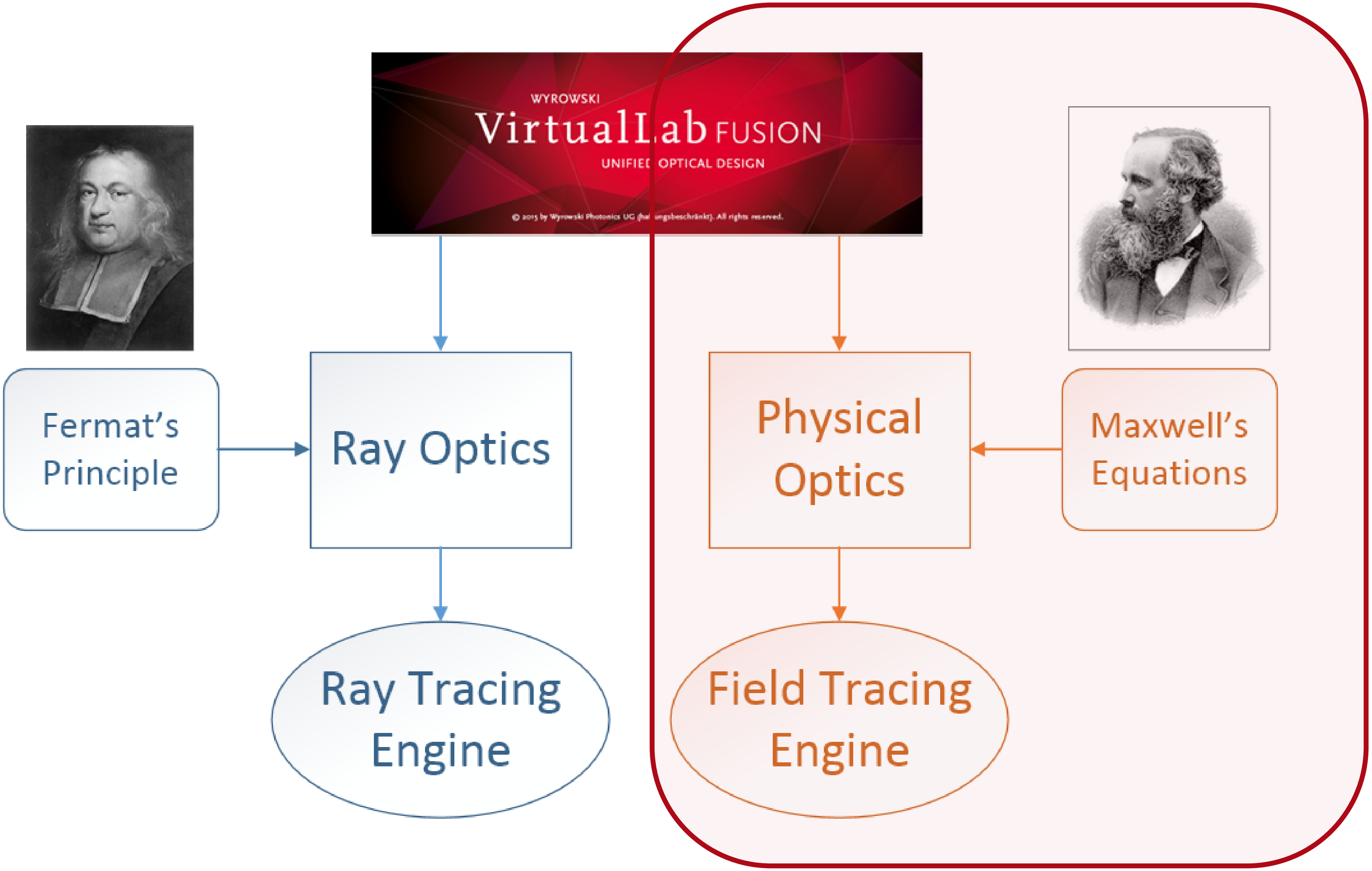
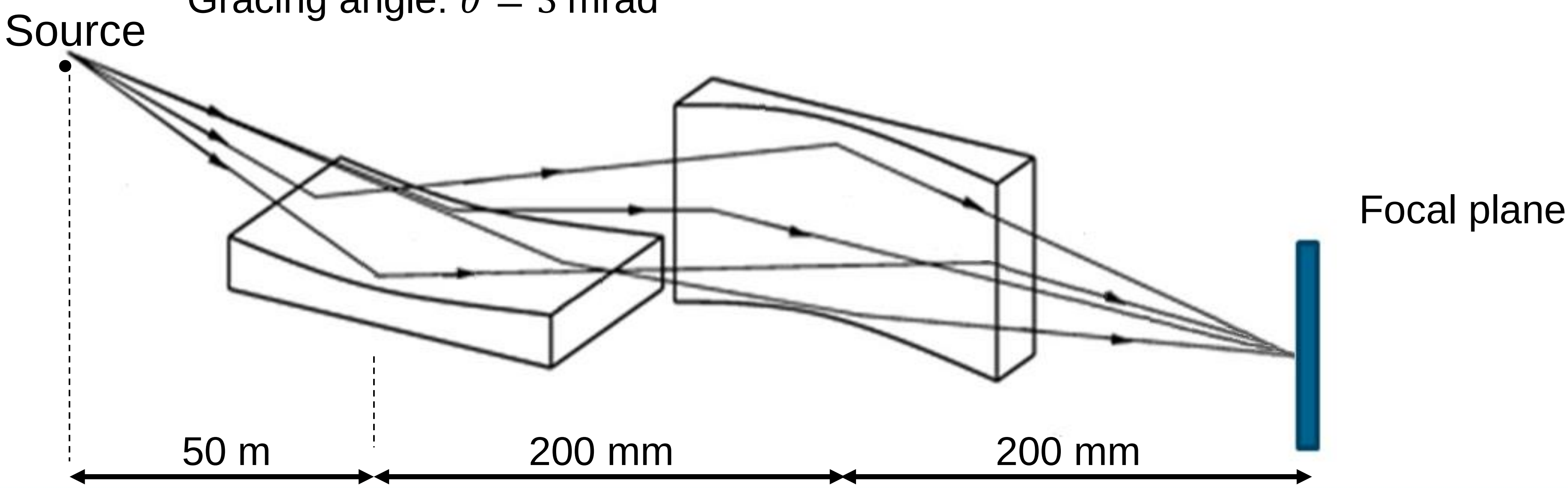


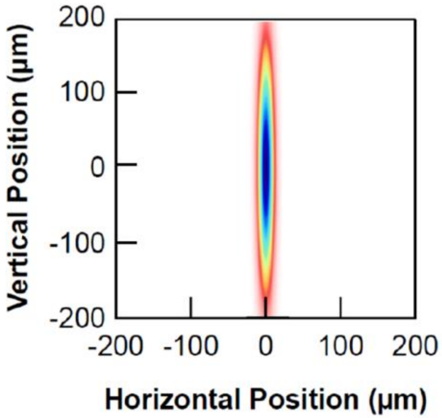
System Modeling Example #1 Provided by Mourad Idir, BNL

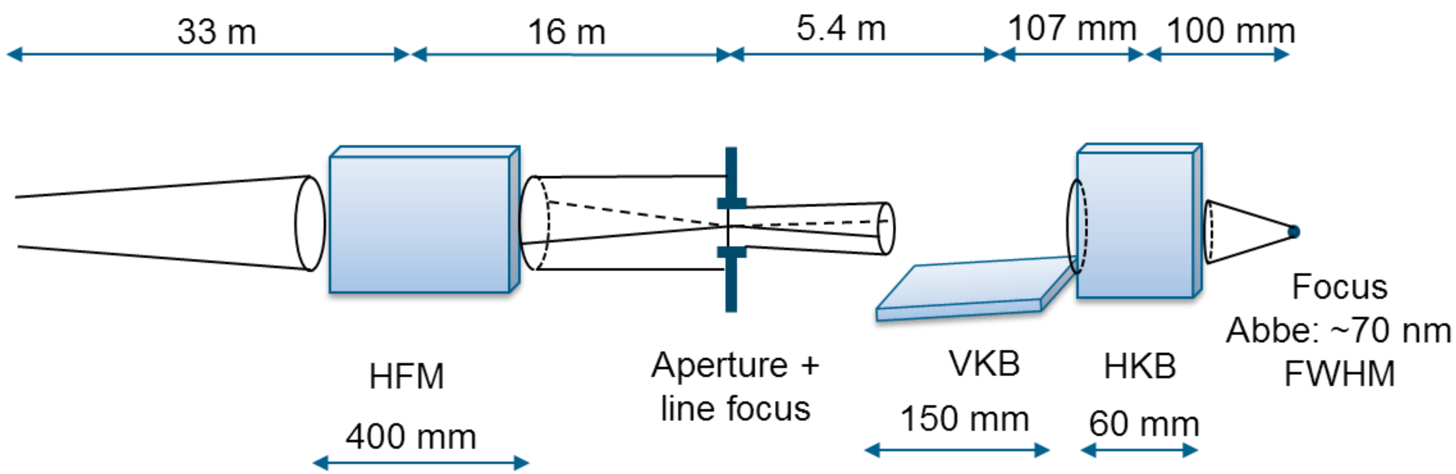
- Source
  - λ = 0.1 nm, 12 keV
  - Spherical wave, fully coherent field
  - 50 m to mirror,12 µrad opening angle
- Mirrors
  - Elliptical, focal points at source & focal plane
  - Gracing angle: $\theta = 3$ mrad



System Modeling Example #2 Provided by Mourad Idir, BNL

- Source
  - λ = 0.173 nm, 7.18 keV
  - Partially coherent field:
    - Gaussian shape profile
    - Size: Δx = 22 µm, Δy = 548 µm
    - Divergence: θ_x = 12.4 µrad, θ_y = 24.8 µrad





Physical Optics Modeling: Source

- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent source field **modes**.
- The representation of source fields by modes enables modeling of
  - Fully coherent source fields
  - Partially spatially coherent source fields
  - Partially temporally coherent source fields
  - Ultrashort pulsed source fields
- Electromagnetic source field modes are determined by six field components of the **E** and **H**-field. That includes automatically
  - Energy quantities
  - Wavefront (phase)
  - Polarization
  - Degrees of coherence and polarization
  - Pulsed field characteristics

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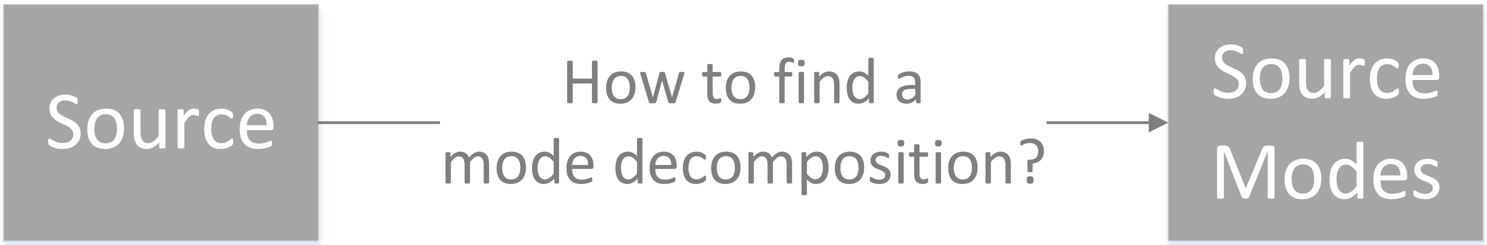

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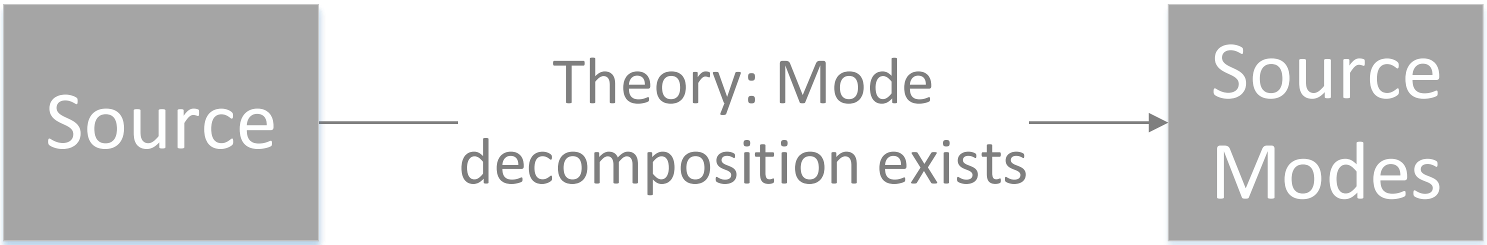

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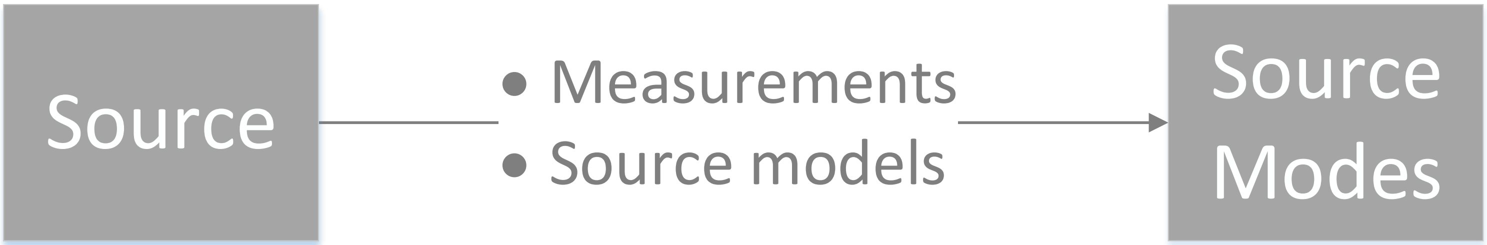

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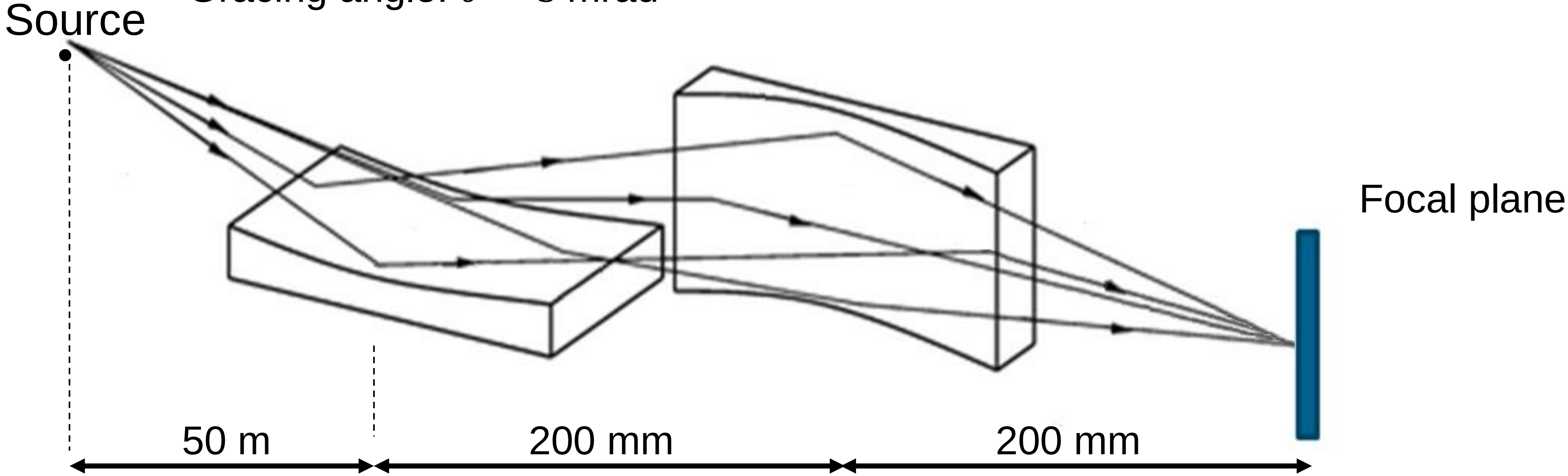
One spherical field mode with 12 µrad opening angle



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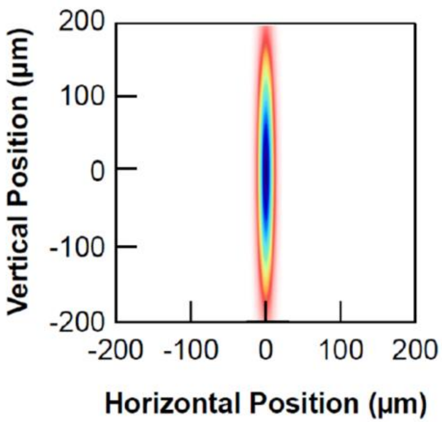

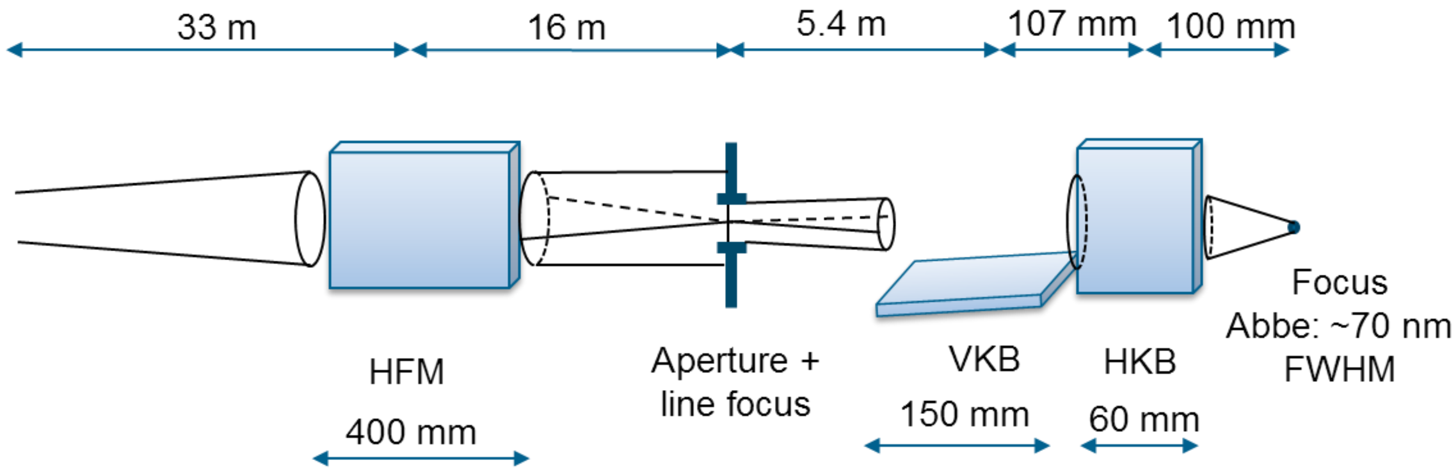

Elementary Shifted Mode Concept

- For extended, quasihomogeneous sources like LED and synchrotron radiation the elementary shifted mode concept is reasonable.

Finite-elementary-source model for partially coherent radiation

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P. Vahimaa and J. Turunen, *Opt. Express* **14,** 1376–1381 (2006).

2004 J. Opt. Soc. Am. A/Vol. 27, No. 9/September 2010 Tervo *et al.*

Shifted-elementary-mode representation for partially coherent vectorial fields

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Corresponding author: jani.tervo@joensuu.fi

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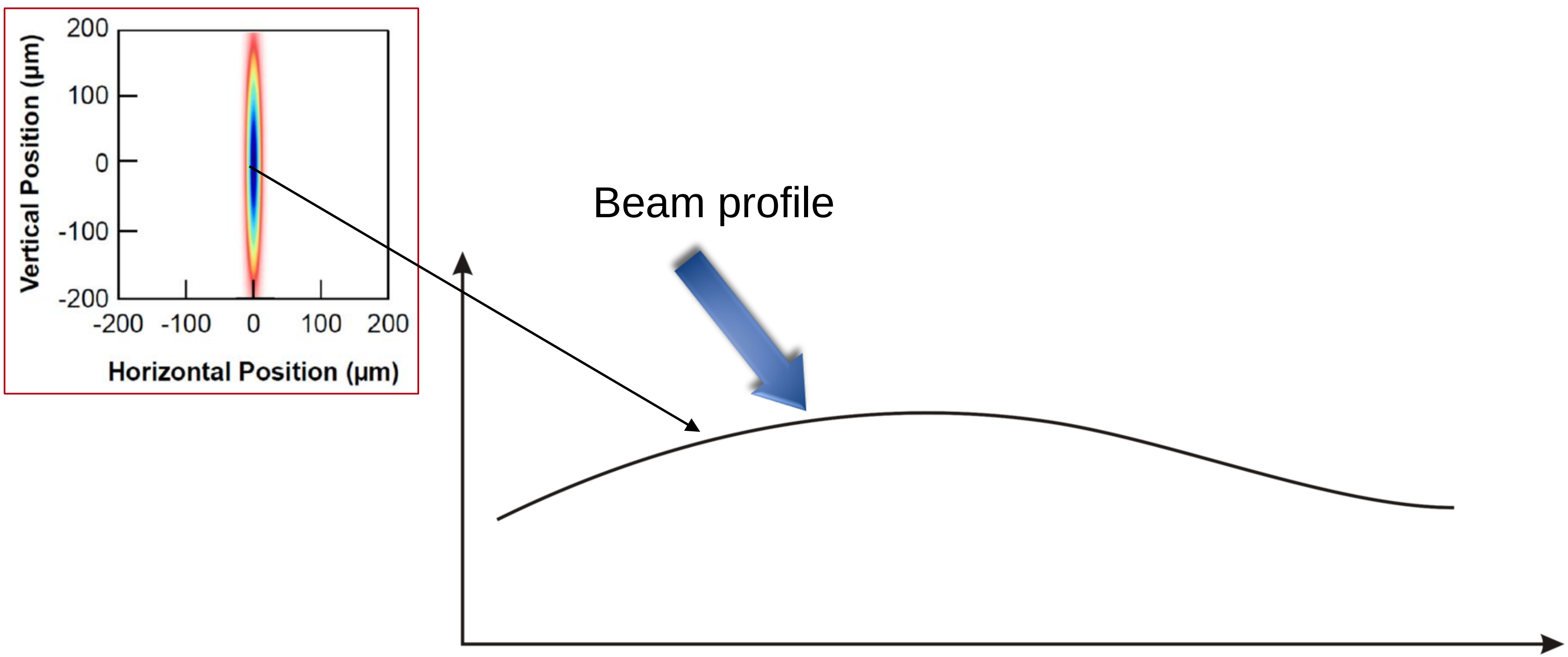

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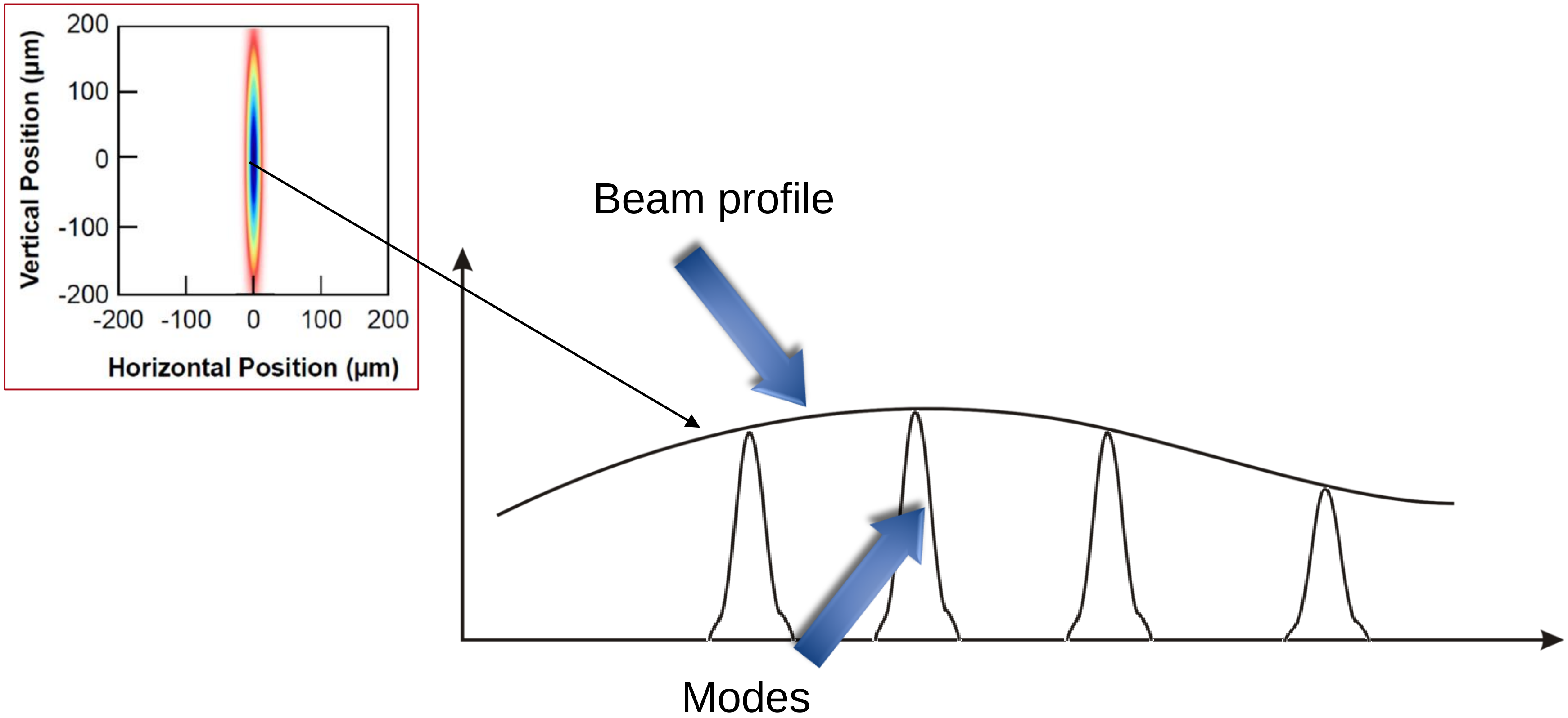

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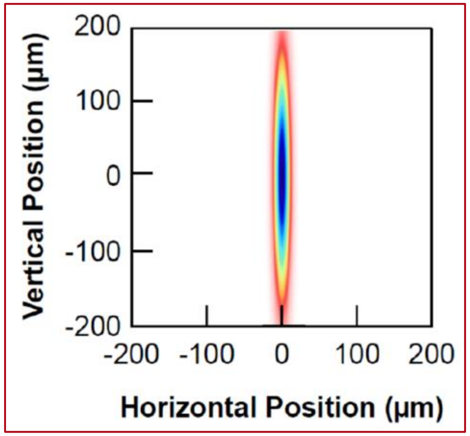

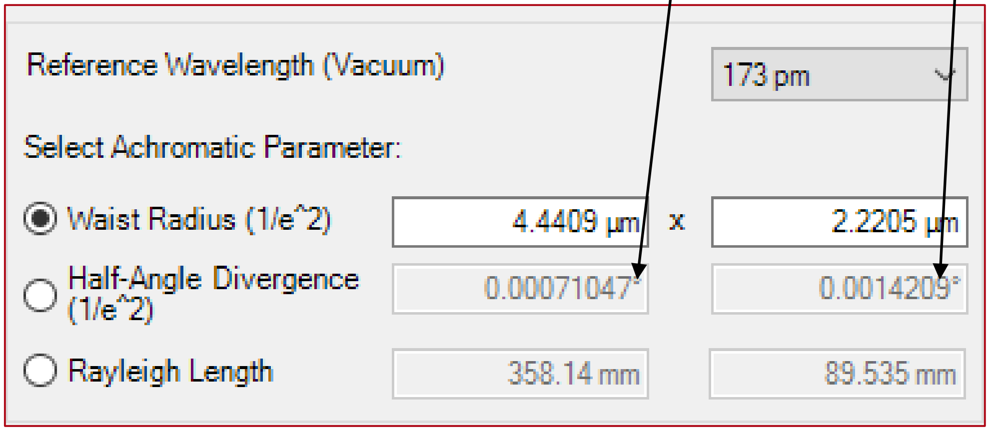

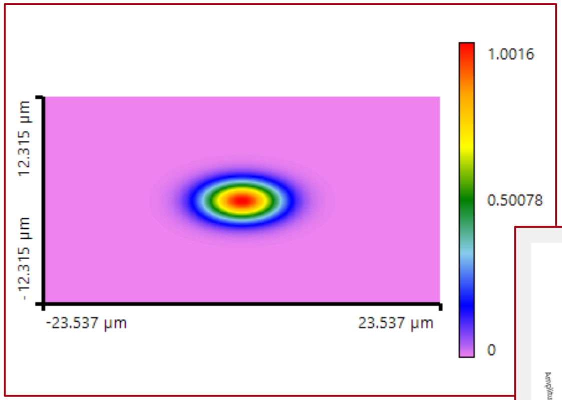

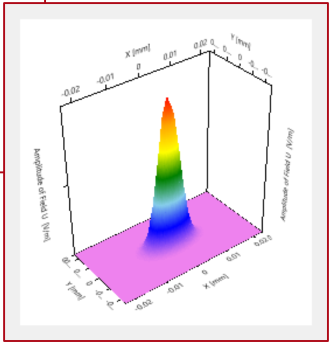

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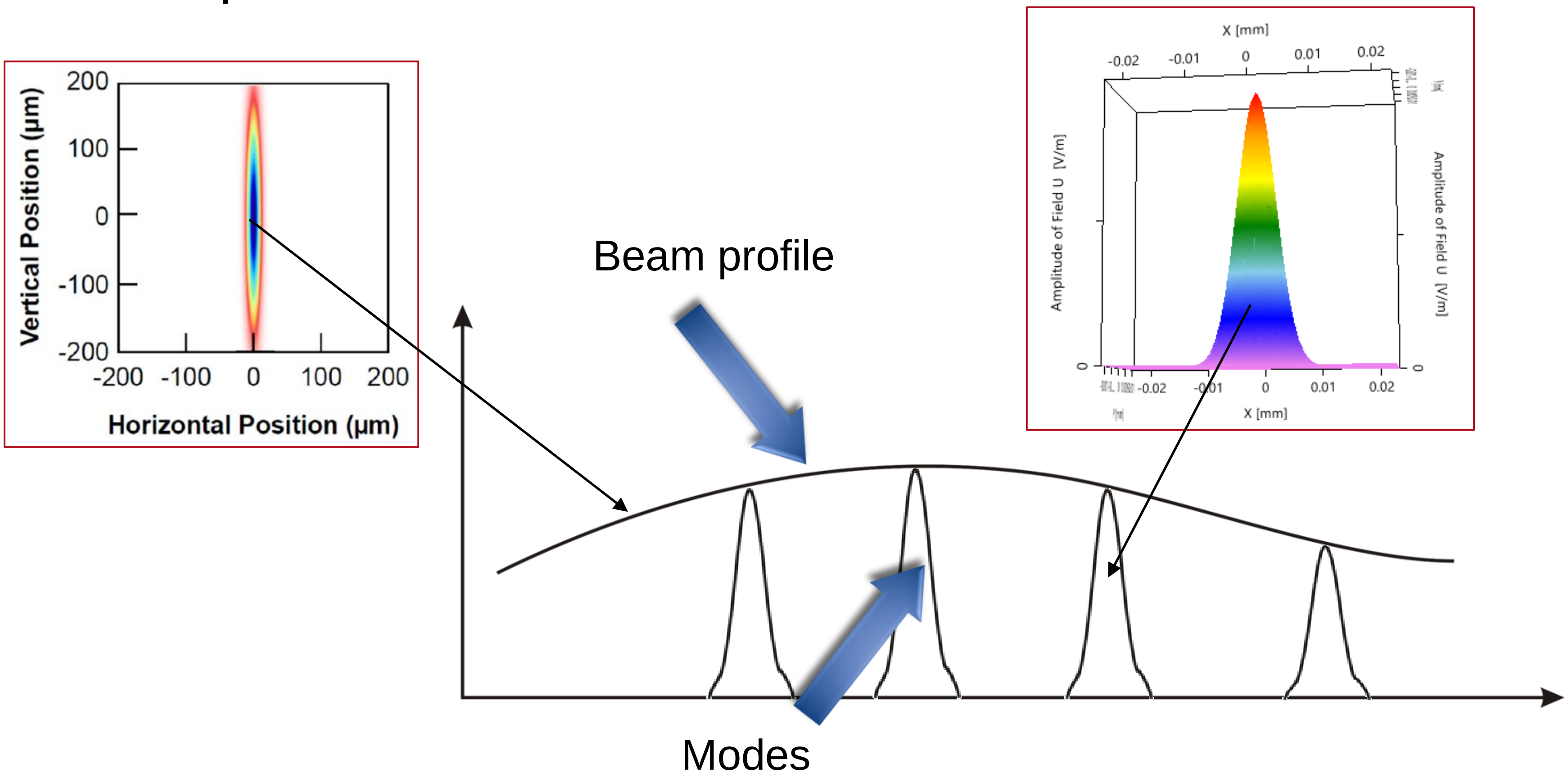

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- The representation of source fields by modes enables modeling of
  - Fully coherent source fields
  - Partially spatially coherent source fields
  - Partially temporally coherent source fields
  - **Ultrashort pulsed source fields**
- Pulses are modeled by a Fourier decomposition of the temporal function, which results in a set of mutually coherent monochromatic source field modes.
- VirtualLab provides 3D modeling of any type of laterally and temporally pulsed field shape.

Physical Optics Modeling: System

- **Source modeling:** Representation of source field in input plane of system by set of monochromatic, fully coherent fields.
- **System modeling:** Sequential or non-sequential propagation of source field modes through system including
  - Free-space propagation
  - Mirrors and lenses; any type of smooth surfaces
  - Surfaces with multilayered stacks
  - Gratings
  - Surfaces with microstructured stacks, e.g. Zone plate
  - Capillary optics
  - … and whatever component the application might require

➡ VirtualLab enables to tackle all those physical optics modeling challenges!

Physical Optics Modeling: System

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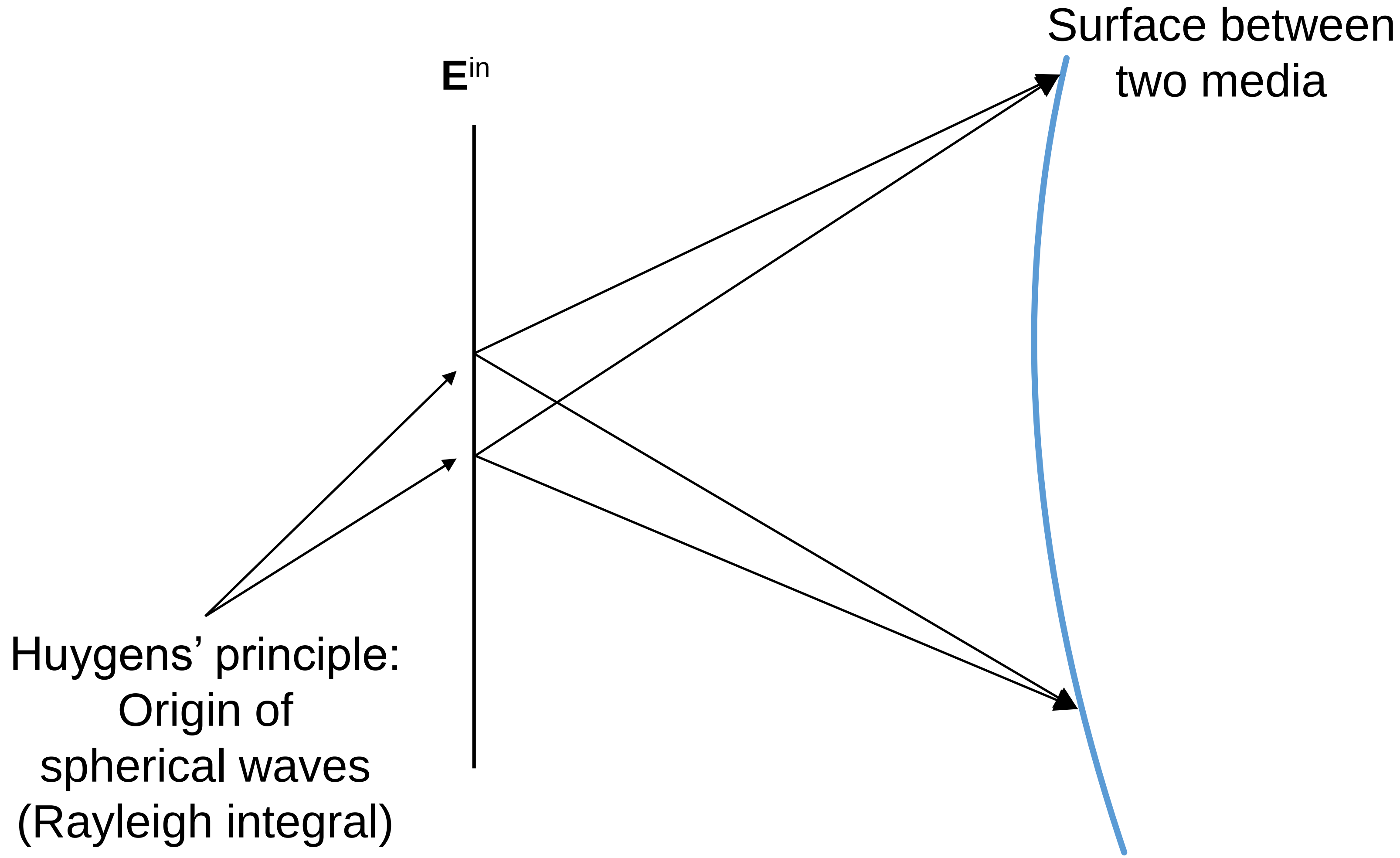
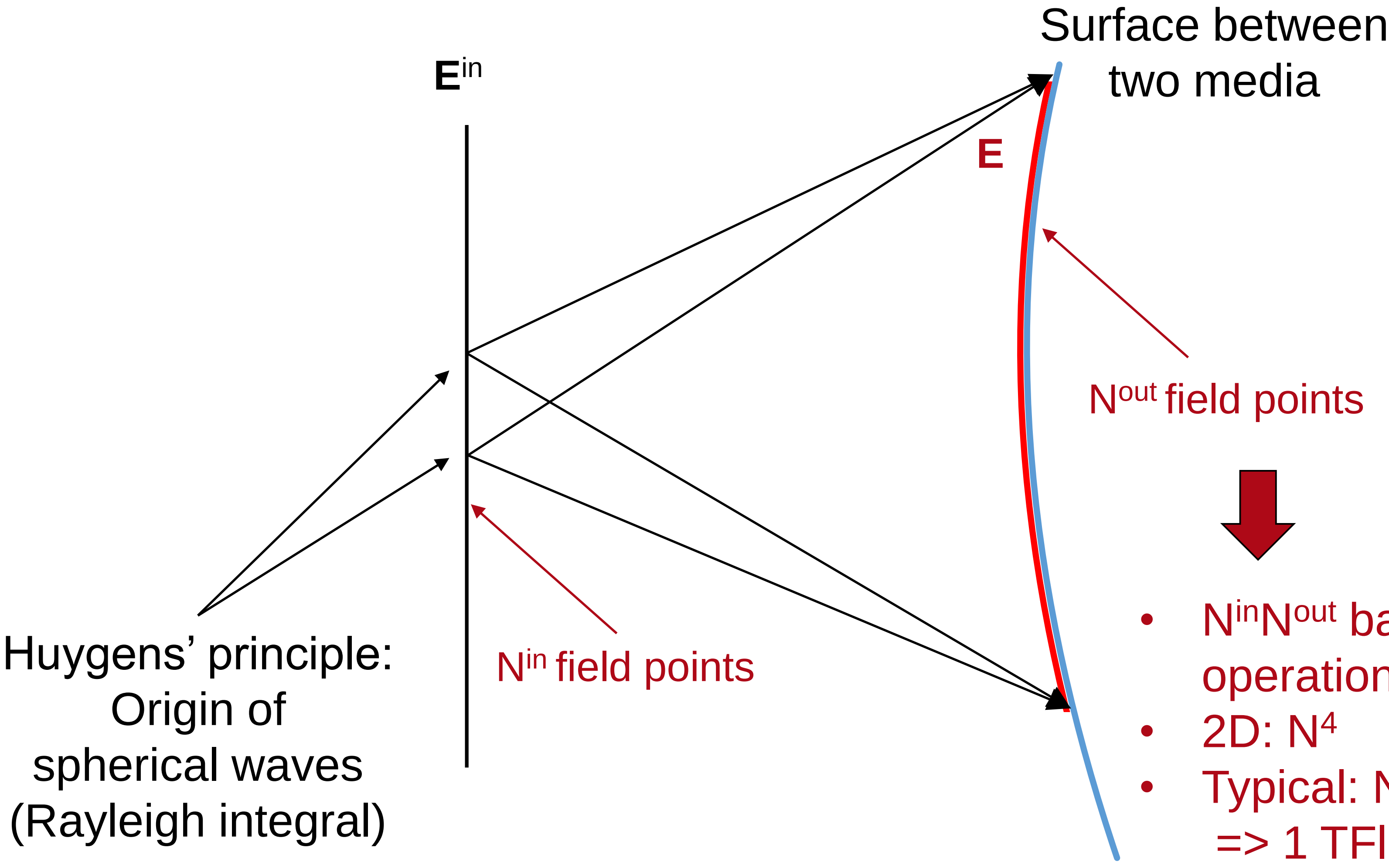
Physical optics modeling is considered to be slowly compared to ray tracing. Is that really true?

Basic Modeling Situation

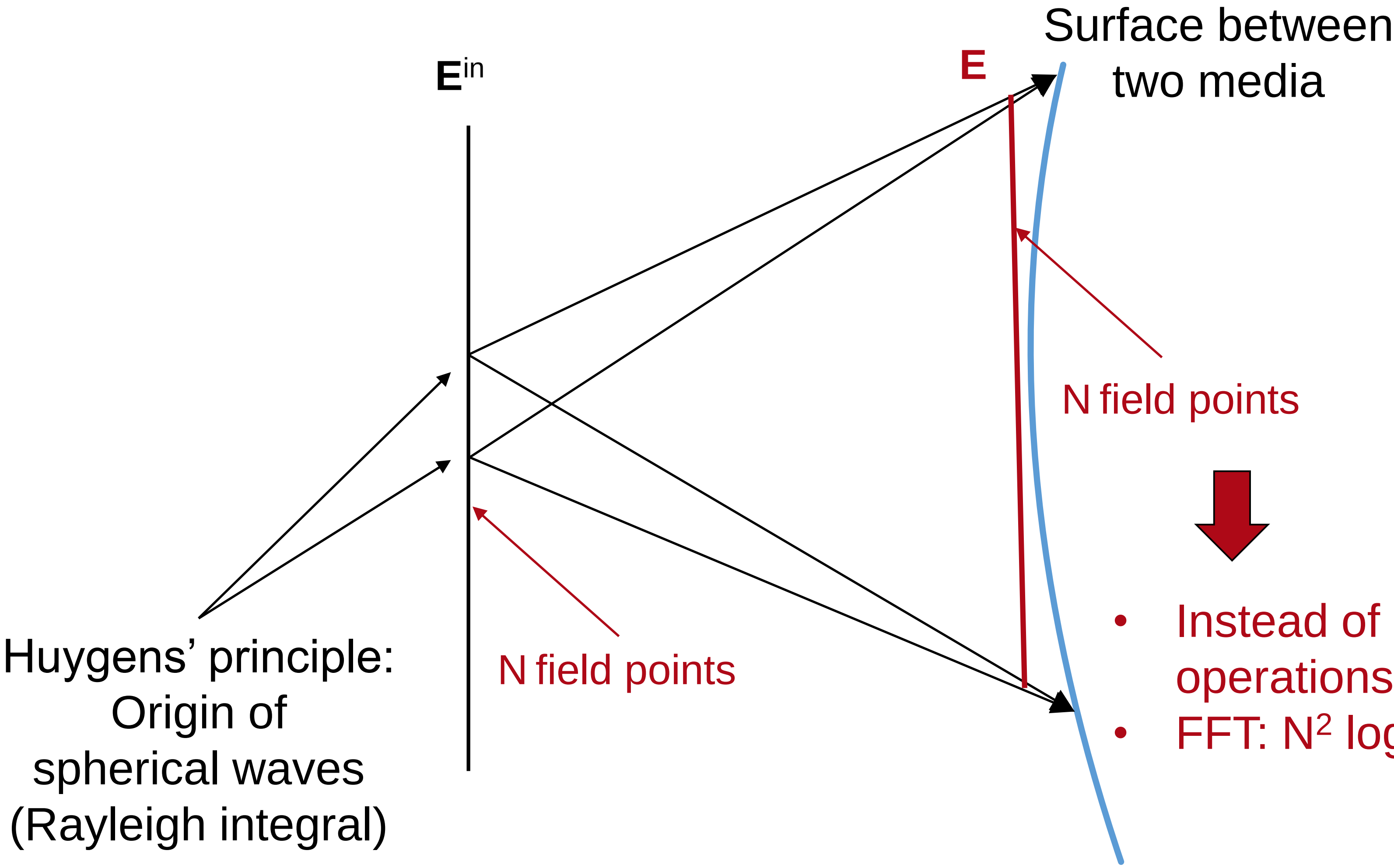


Basic Modeling Situation



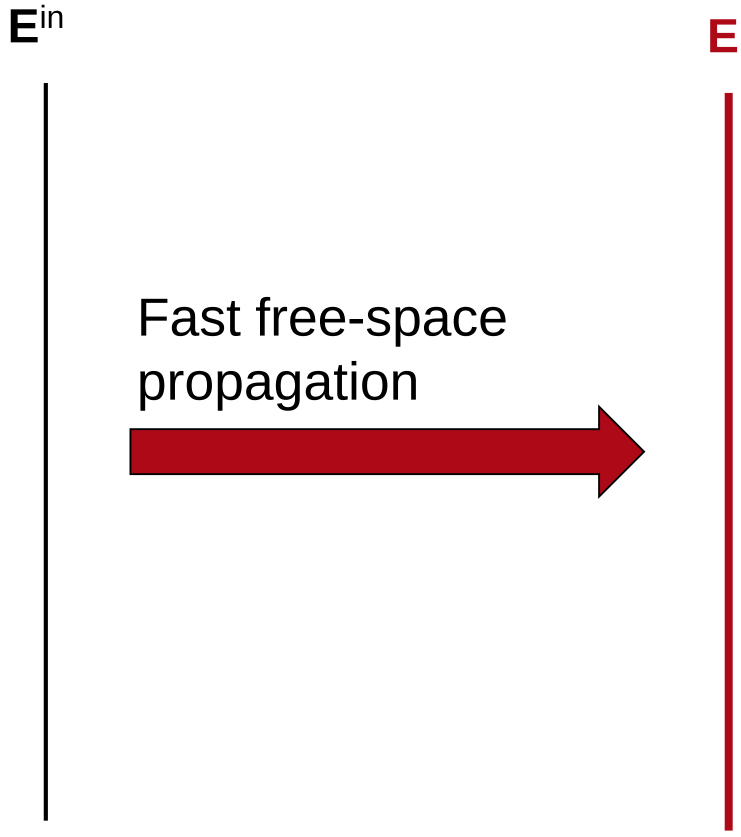
- $N^{in}N^{out}$ basic operations
- 2D: N^4
- Typical: N=1000 => 1 TFlop

Propagation by FFT Techniques

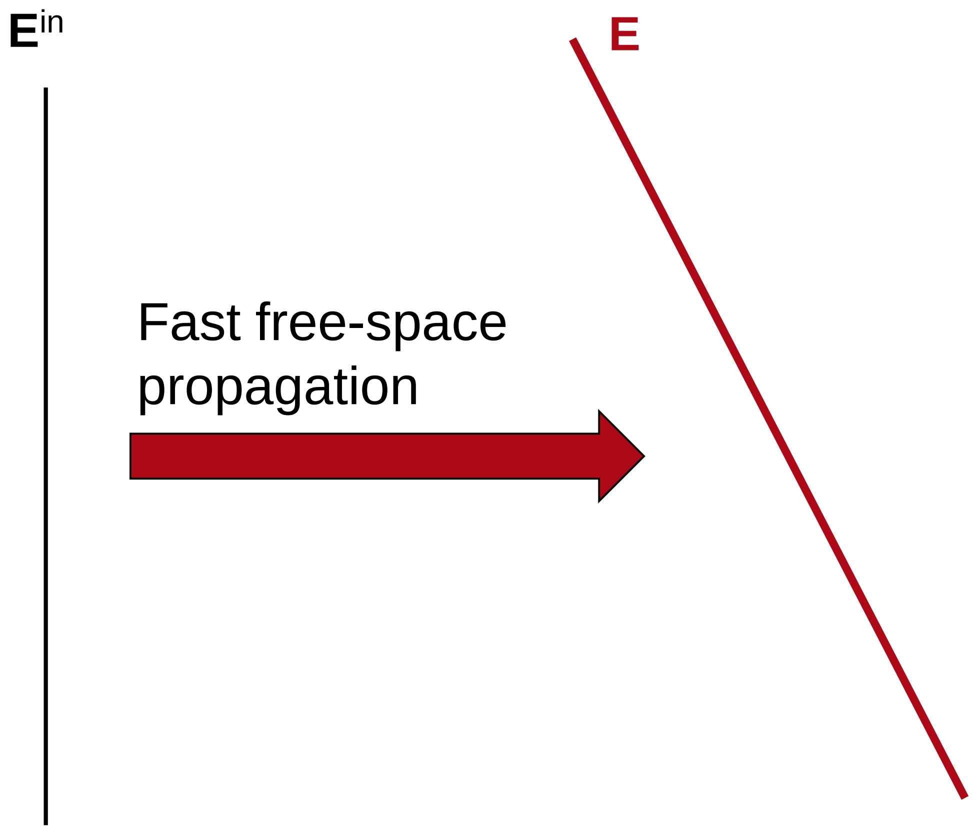


- Instead of N^4 operations
- FFT: $N^2 \log N$

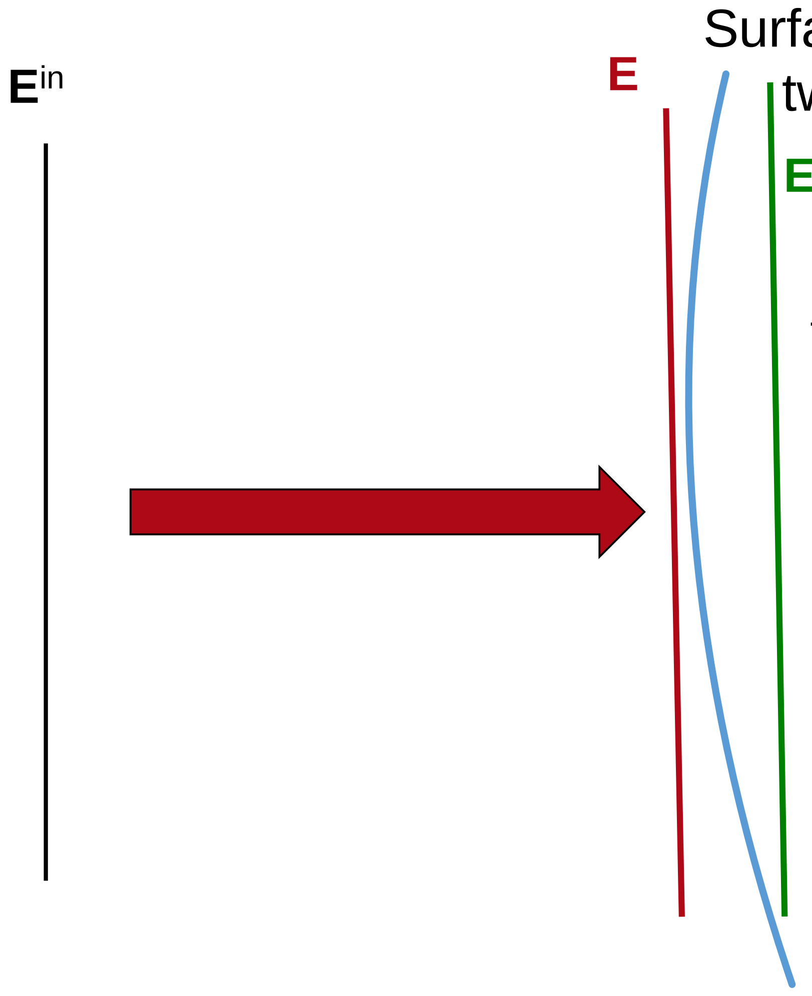
Propagation by FFT Techniques



Propagation by FFT Techniques



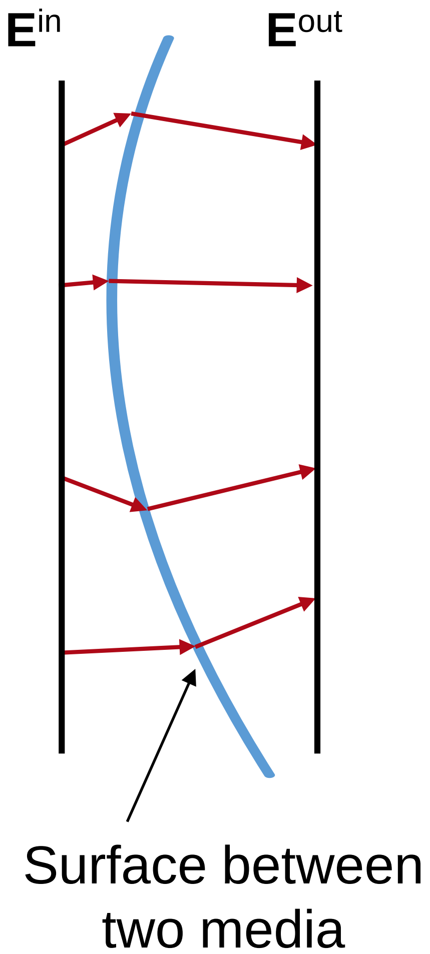
Basic Modeling Situation: Boundary Problem



How to obtain the transmitted and reflected fields?

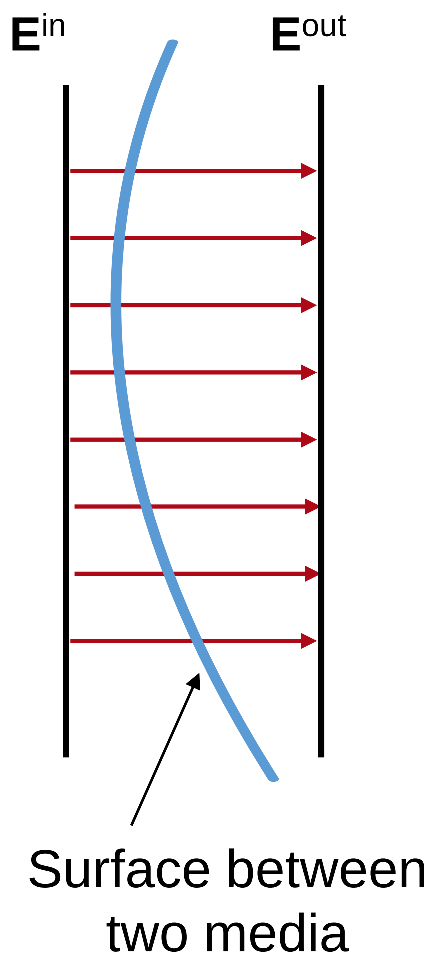
How to solve boundary value problem?

Geometric Field Tracing through Surface



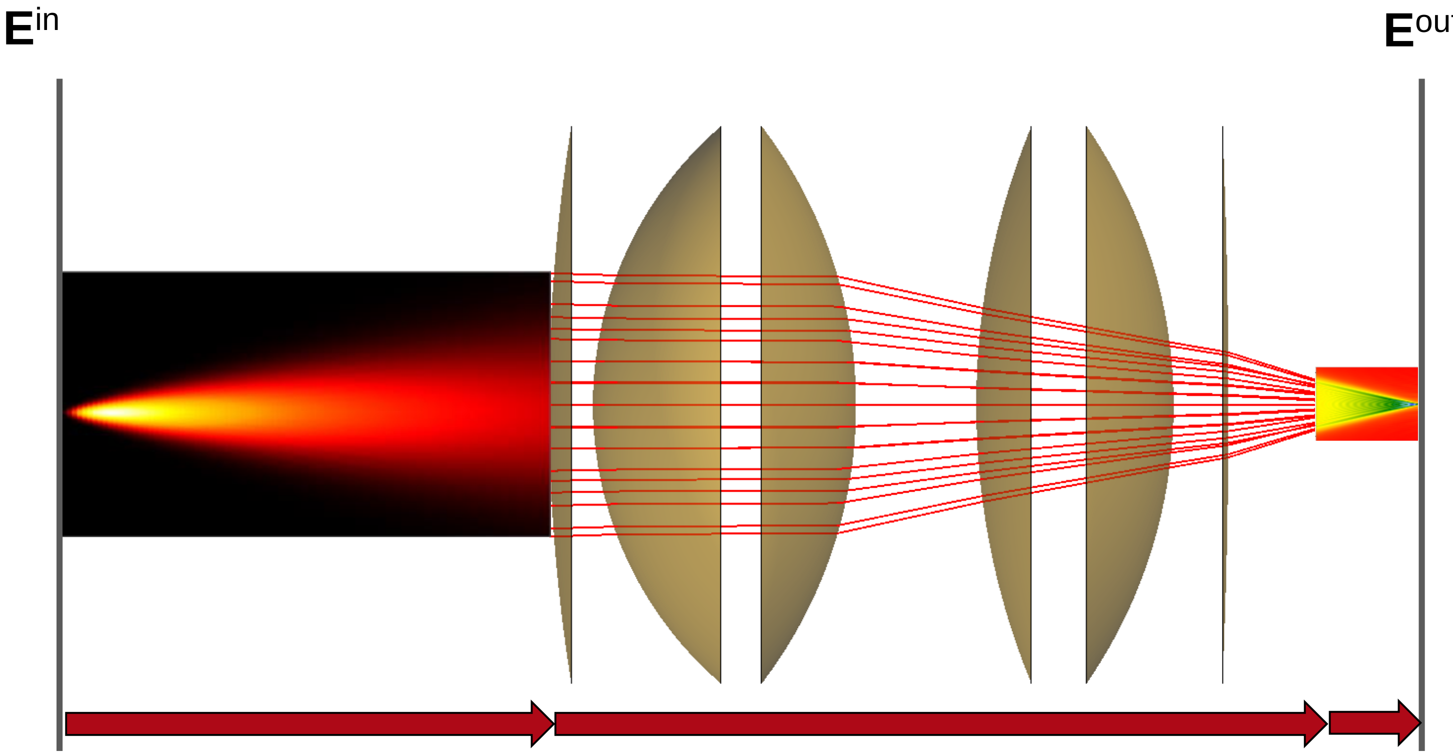
- Input field is decomposed into local plane wave fields.
- That is theoretically justified if field is in its geometric zone.
- Local plane waves (smart rays) are propagated through surface by local application of plane wave/plane surface interaction (law of refraction and Fresnel’s equations).
- By including all vectorial effects and considering intensity law of geometrical optics the output field can be constructed.

Paraxial Modeling of Surfaces



- In paraxial optics the local plane waves propagate all along the axis and the deflection at the surface by refraction is neglected.
- Then just the optical path length is considered and a phase term proportional to the height profile is obtained.
- That is the thin element approximation (TEA) frequently used in paraxial optics, e.g. Fourier and laser optics.
- Together with Fresnel integral for free-space propagation the Collins integral follows for lens systems.

Fast Physical Optics Modeling



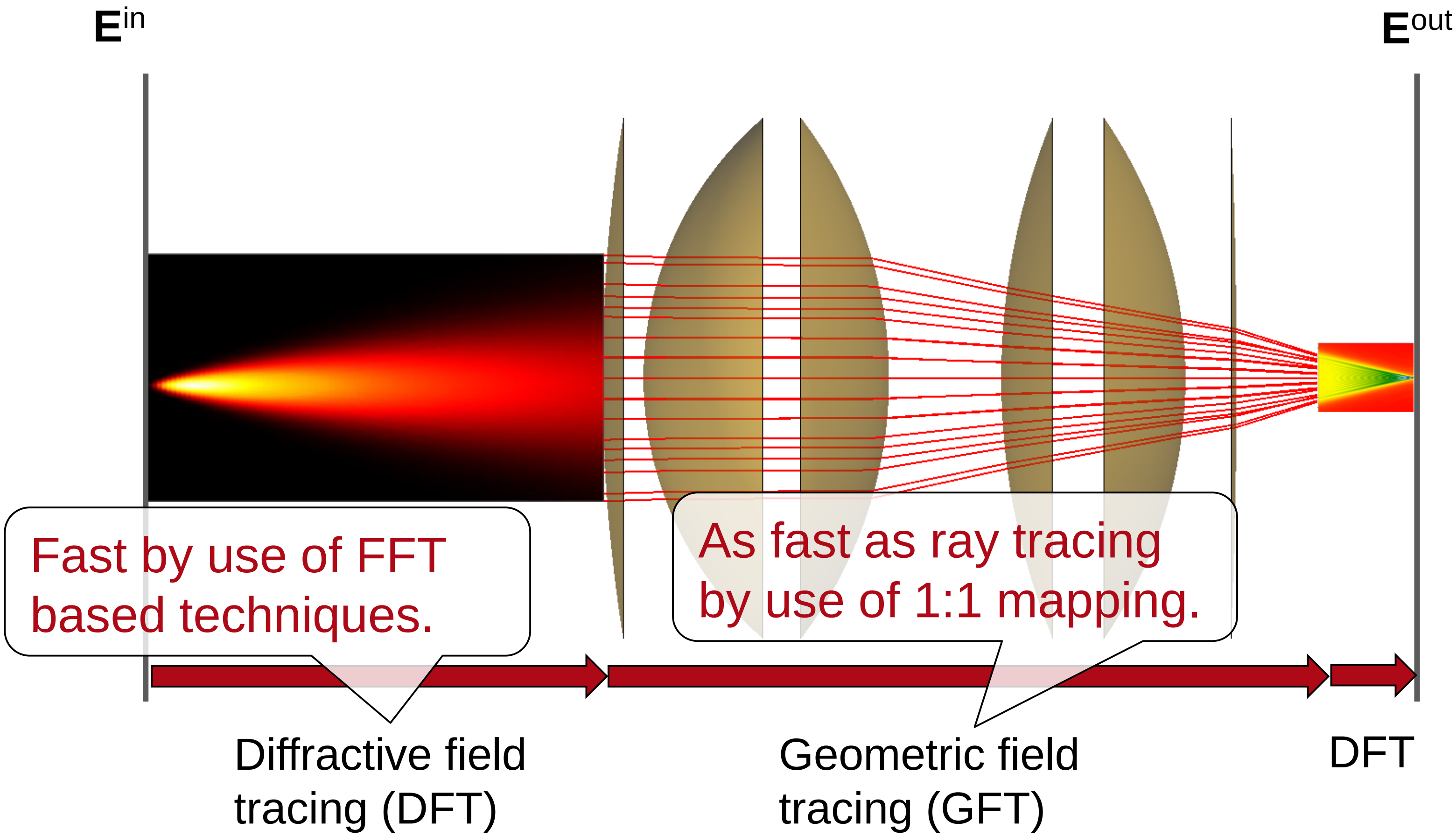
Diffractive field tracing (DFT)

Geometric field tracing (GFT)

DFT

Field must be always in its geometric zone!

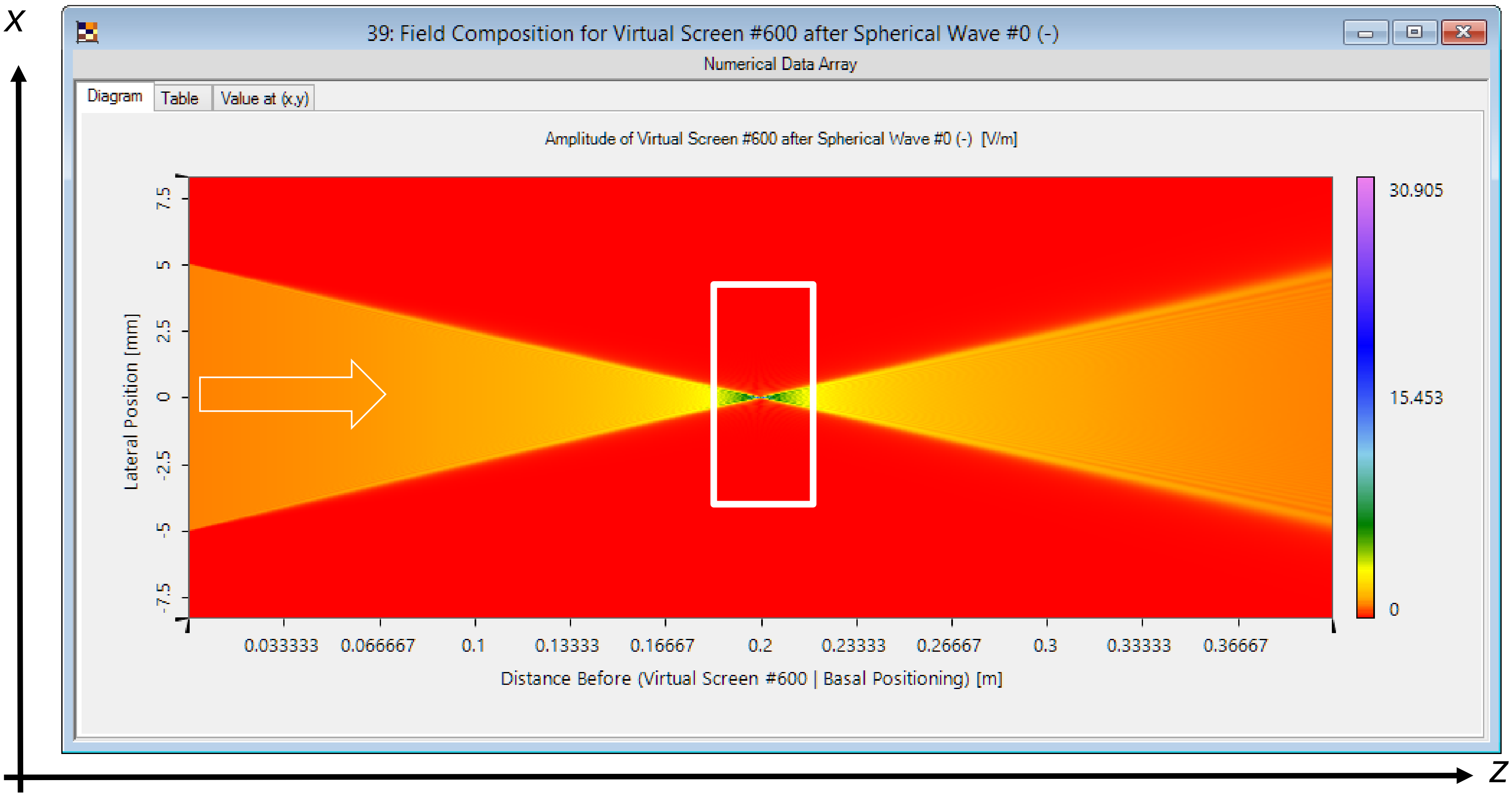
Fast Physical Optics Modeling



Field must be always in its geometric zone!

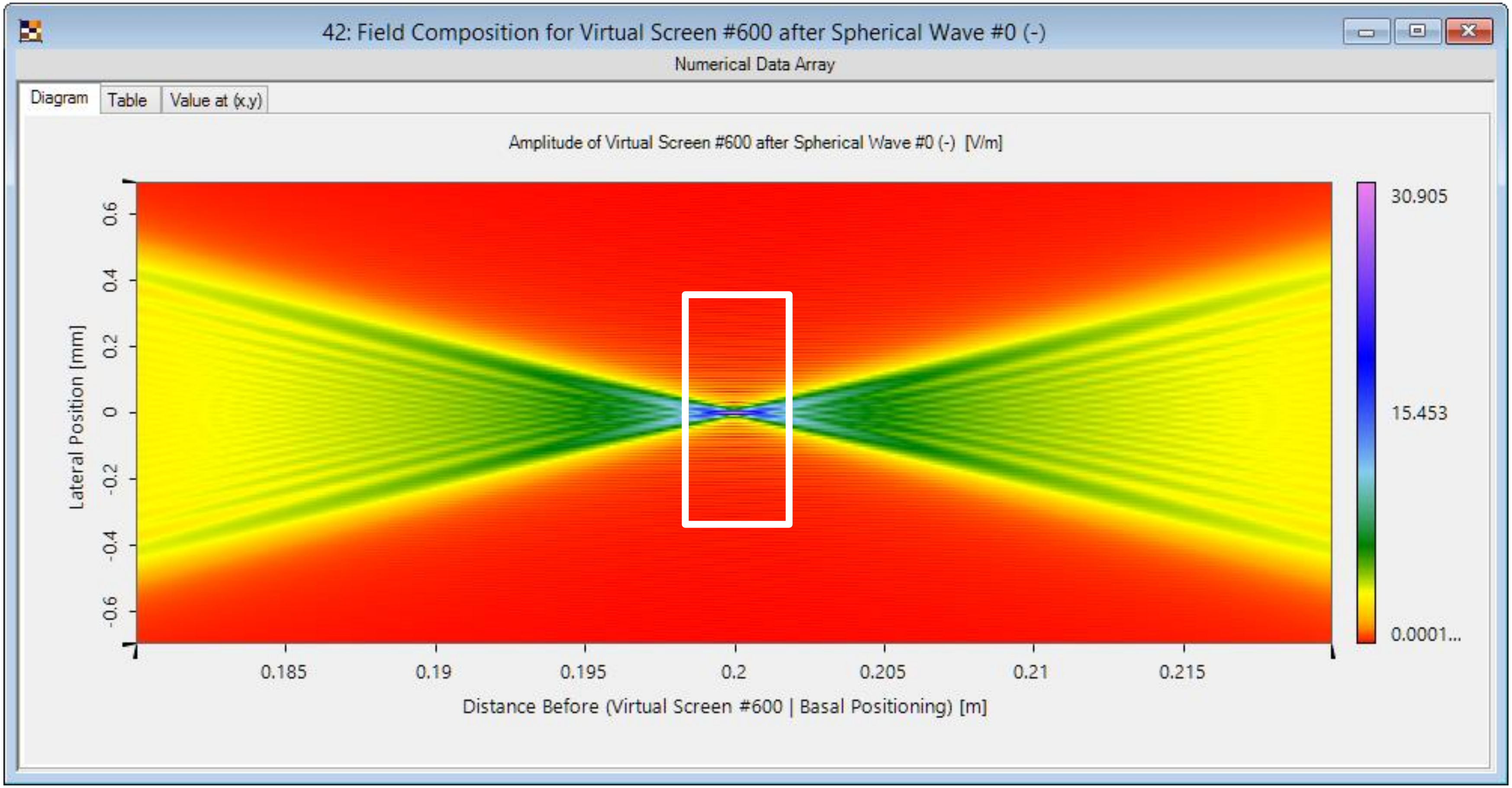
Spherical Wave: f = 200 mm; z= 0 - 400mm

Field propagated along the z-axis



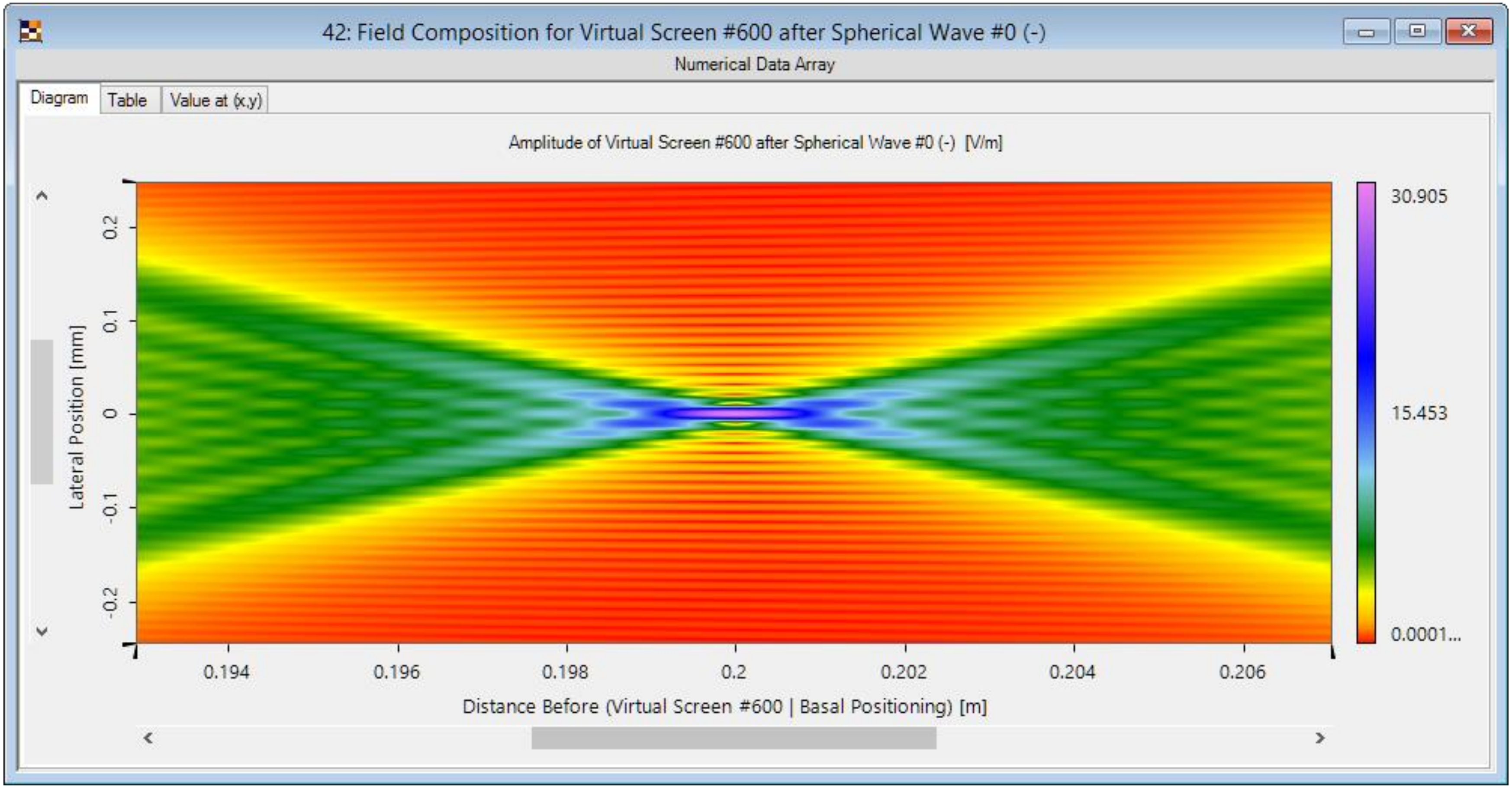
Spherical Wave: f = 200 mm; z= 180 – 220 mm

Field propagated along the z-axis



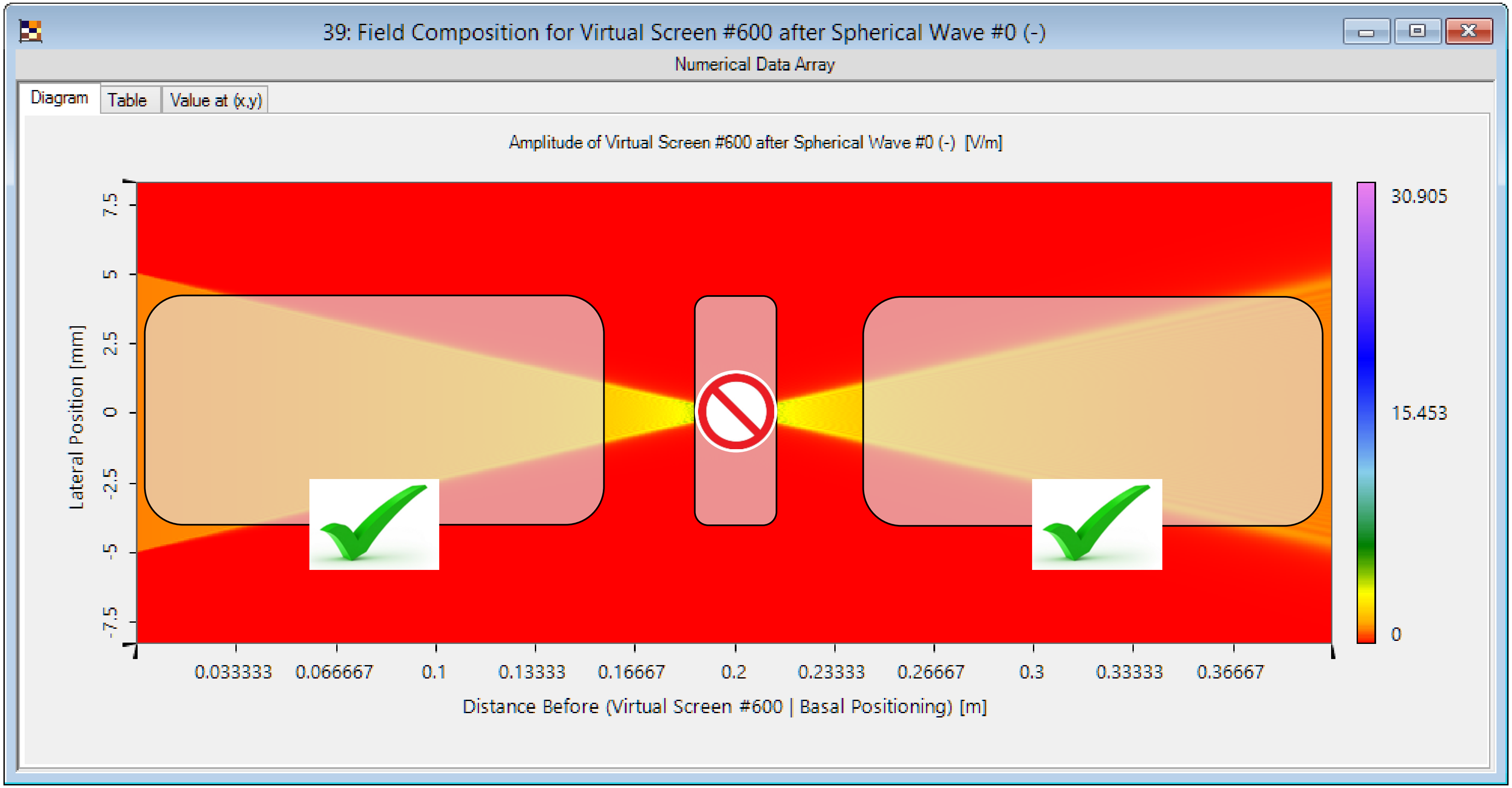
Spherical Wave: f = 200 mm; z= 193 – 207 mm

Field propagated along the z-axis

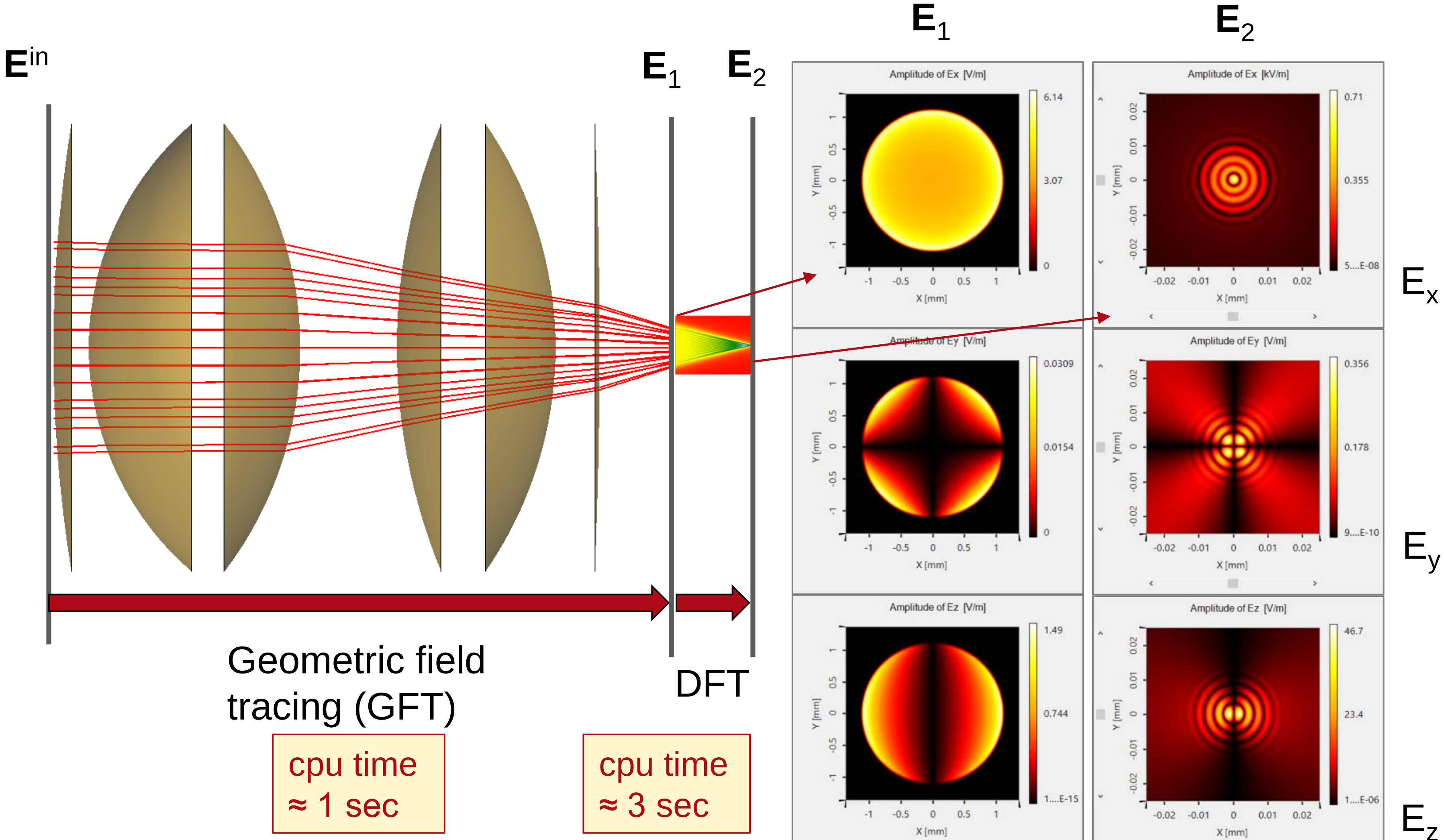


Spherical Wave: Geometric Zone?

Field propagated along the z-axis

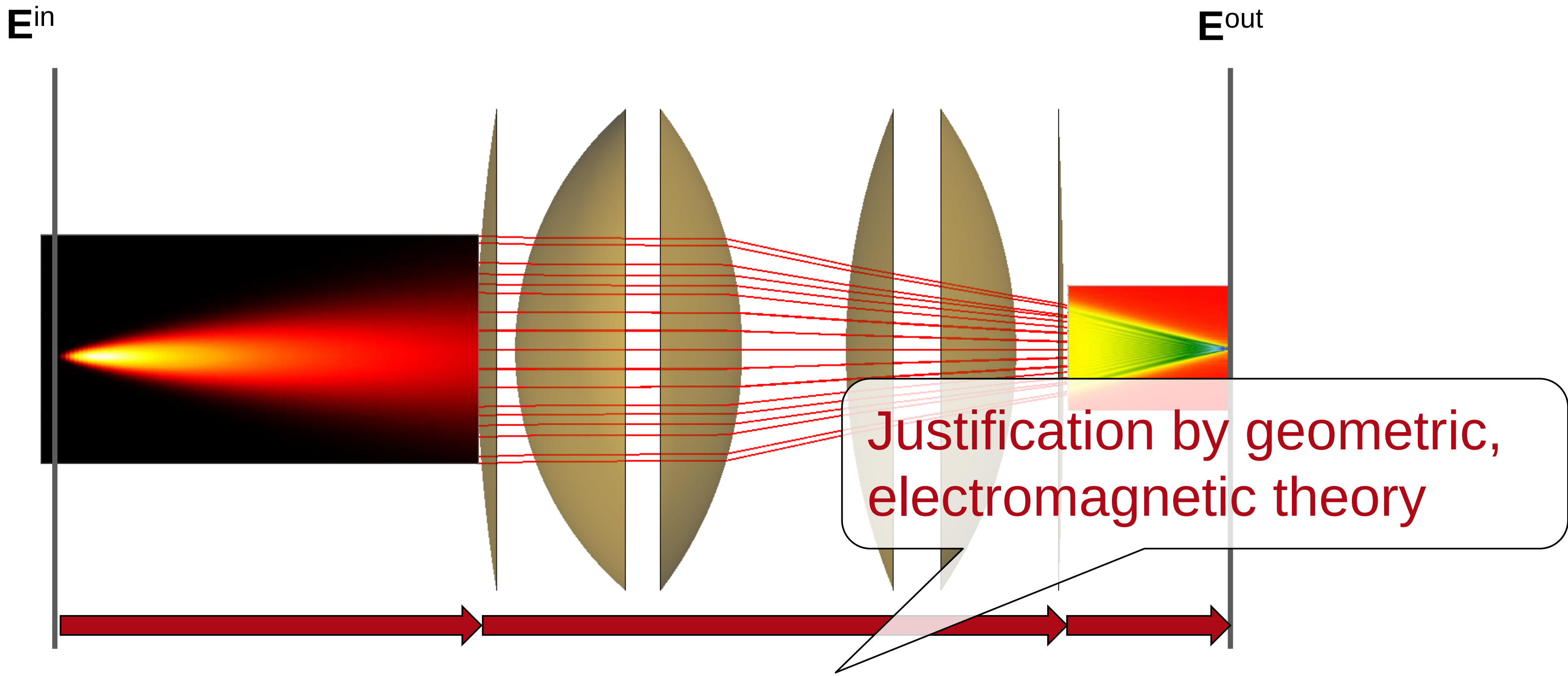


Fast Physical Optics Modeling: Example



cpu time an standard laptop

Fast Physical Optics Modeling



Diffractive field tracing (DFT)

Geometric field tracing (GFT)

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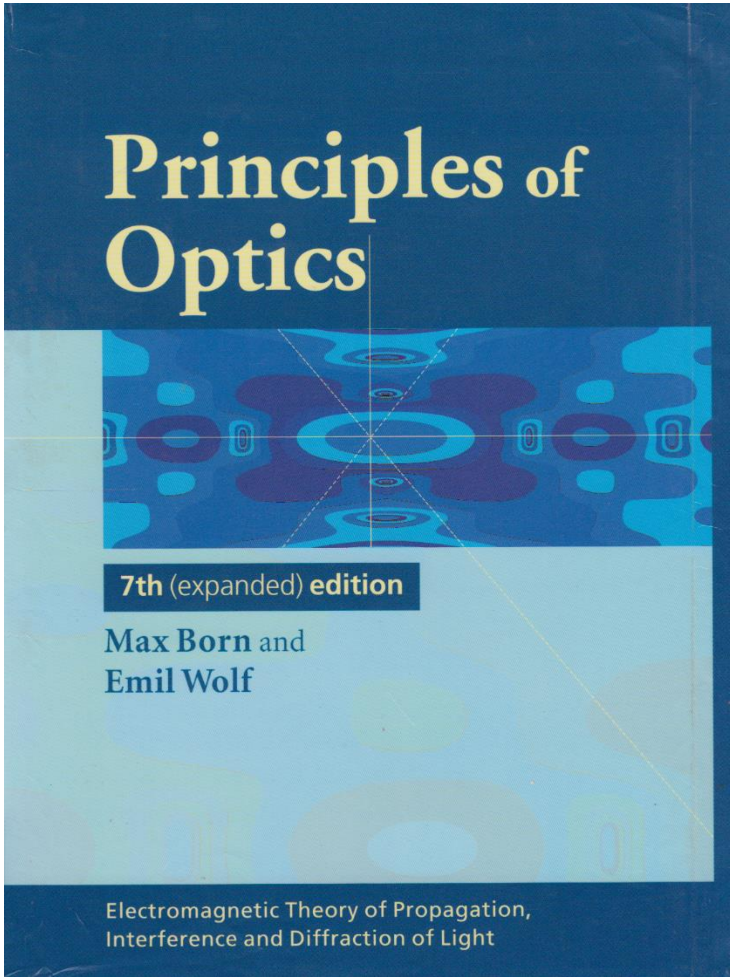
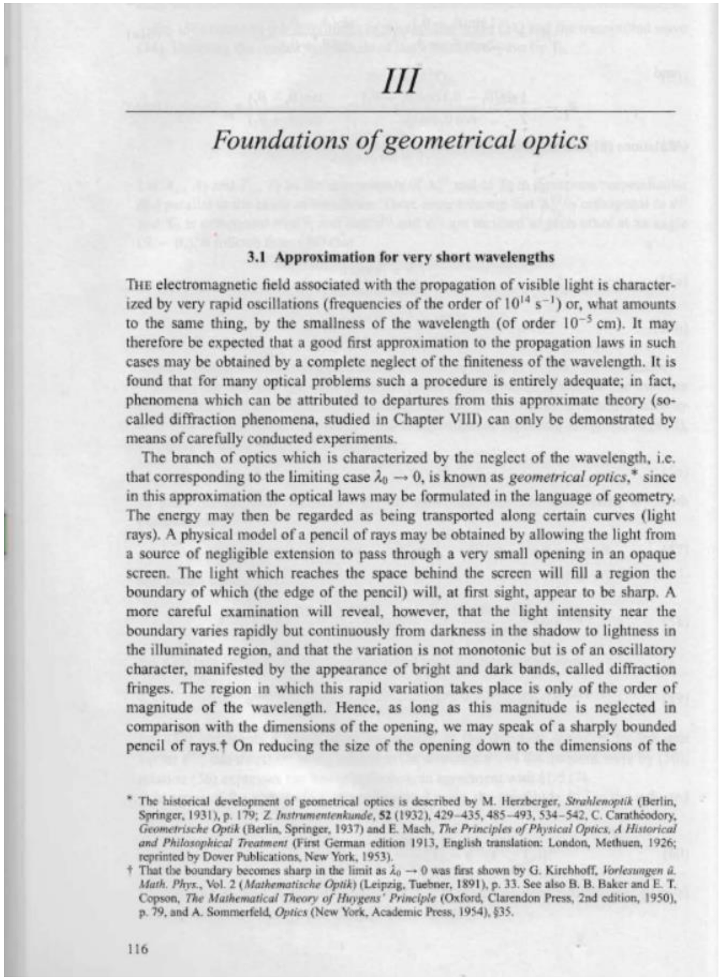
Field must be always in its geometric zone!

Geometrical Optics of Electromagnetic Fields





III

Foundations of geometrical optics

3.1 Approximation for very short wavelengths

The electromagnetic field associated with the propagation of visible light is characterized by very rapid oscillations (frequencies of the order of 10^{14} s^{-1}) or, what amounts to the same thing, by the smallness of the wavelength (of order 10^{-5} cm). It may therefore be expected that a good first approximation to the propagation laws in such cases may be obtained by a complete neglect of the finiteness of the wavelength. It is found that for many optical problems such a procedure is entirely adequate; in fact, phenomena which can be attributed to departures from this approximate theory (so-called diffraction phenomena, studied in Chapter VIII) can only be demonstrated by means of carefully conducted experiments.

The branch of optics which is characterized by the neglect of the wavelength, i.e. that corresponding to the limiting case $\lambda_0 \rightarrow 0$, is known as *geometrical optics*,* since in this approximation the optical laws may be formulated in the language of geometry. The energy may then be regarded as being transported along certain curves (light rays). A physical model of a pencil of rays may be obtained by allowing the light from a source of negligible extension to pass through a very small opening in an opaque screen. The light which reaches the space behind the screen will fill a region the boundary of which (the edge of the pencil) will, at first sight, appear to be sharp. A more careful examination will reveal, however, that the light intensity near the boundary varies rapidly but continuously from darkness in the shadow to lightness in the illuminated region, and that the variation is not monotonic but is of an oscillatory character, manifested by the appearance of bright and dark bands, called diffraction fringes. The region in which this rapid variation takes place is only of the order of magnitude of the wavelength. Hence, as long as this magnitude is neglected in comparison with the dimensions of the opening, we may speak of a sharply bounded pencil of rays.† On reducing the size of the opening down to the dimensions of the

* The historical development of geometrical optics is described by M. Herzberger, *Strahlenoptik* (Berlin, Springer, 1931), p. 179; *Z. Instrumentenkunde*, **52** (1932), 429–435, 485–493, 534–542, C. Carathéodory, *Geometrische Optik* (Berlin, Springer, 1937) and E. Mach, *The Principles of Physical Optics, A Historical and Philosophical Treatment* (First German edition 1913, English translation: London, Methuen, 1926; reprinted by Dover Publications, New York, 1953).

† That the boundary becomes sharp in the limit as $\lambda_0 \rightarrow 0$ was first shown by G. Kirchhoff, *Vorlesungen ü. Math. Phys.*, Vol. 2 (*Mathematische Optik*) (Leipzig, Tuebner, 1891), p. 33. See also B. B. Baker and E. T. Copson, *The Mathematical Theory of Huygens' Principle* (Oxford, Clarendon Press, 2nd edition, 1950), p. 79, and A. Sommerfeld, *Optics* (New York, Academic Press, 1954), §35.

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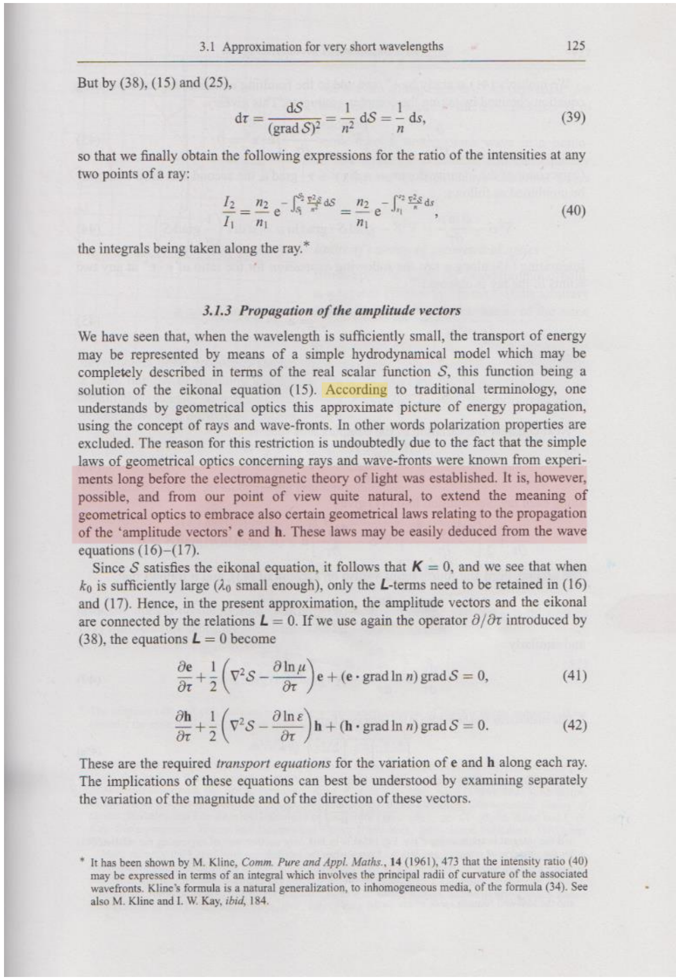
Geometrical Optics of Electromagnetic Fields



3.1 Approximation for very short wavelengths 125

But by (38), (15) and (25),

$$d\tau = \frac{d\mathcal{S}}{(\operatorname{grad}\mathcal{S})^2} = \frac{1}{n^2}\,d\mathcal{S} = \frac{1}{n}\,ds, \tag{39}$$

so that we finally obtain the following expressions for the ratio of the intensities at any two points of a ray:

$$\frac{I_2}{I_1} = \frac{n_2}{n_1}\,e^{-\int_{\mathcal{S}_1}^{\mathcal{S}_2}\frac{\nabla^2\mathcal{S}}{n^2}d\mathcal{S}} = \frac{n_2}{n_1}\,e^{-\int_{s_1}^{s_2}\frac{\nabla^2\mathcal{S}}{n}ds}, \tag{40}$$

the integrals being taken along the ray.*

3.1.3 *Propagation of the amplitude vectors*

We have seen that, when the wavelength is sufficiently small, the transport of energy may be represented by means of a simple hydrodynamical model which may be completely described in terms of the real scalar function $\mathcal{S}$, this function being a solution of the eikonal equation (15). According to traditional terminology, one understands by geometrical optics this approximate picture of energy propagation, using the concept of rays and wave-fronts. In other words polarization properties are excluded. The reason for this restriction is undoubtedly due to the fact that the simple laws of geometrical optics concerning rays and wave-fronts were known from experiments long before the electromagnetic theory of light was established. It is, however, possible, and from our point of view quite natural, to extend the meaning of geometrical optics to embrace also certain geometrical laws relating to the propagation of the 'amplitude vectors' **e** and **h**. These laws may be easily deduced from the wave equations (16)–(17).

Since $\mathcal{S}$ satisfies the eikonal equation, it follows that $\boldsymbol{K} = 0$, and we see that when k_0 is sufficiently large (λ_0 small enough), only the $\boldsymbol{L}$-terms need to be retained in (16) and (17). Hence, in the present approximation, the amplitude vectors and the eikonal are connected by the relations $\boldsymbol{L} = 0$. If we use again the operator $\partial/\partial\tau$ introduced by (38), the equations $\boldsymbol{L} = 0$ become

$$\frac{\partial\mathbf{e}}{\partial\tau} + \frac{1}{2}\left(\nabla^2\mathcal{S} - \frac{\partial\ln\mu}{\partial\tau}\right)\mathbf{e} + (\mathbf{e}\cdot\operatorname{grad}\ln n)\operatorname{grad}\mathcal{S} = 0, \tag{41}$$

$$\frac{\partial\mathbf{h}}{\partial\tau} + \frac{1}{2}\left(\nabla^2\mathcal{S} - \frac{\partial\ln\varepsilon}{\partial\tau}\right)\mathbf{h} + (\mathbf{h}\cdot\operatorname{grad}\ln n)\operatorname{grad}\mathcal{S} = 0. \tag{42}$$

These are the required *transport equations* for the variation of **e** and **h** along each ray. The implications of these equations can best be understood by examining separately the variation of the magnitude and of the direction of these vectors.

* It has been shown by M. Kline, *Comm. Pure and Appl. Maths.*, **14** (1961), 473 that the intensity ratio (40) may be expressed in terms of an integral which involves the principal radii of curvature of the associated wavefronts. Kline's formula is a natural generalization, to inhomogeneous media, of the formula (34). See also M. Kline and I. W. Kay, *ibid*, 184.

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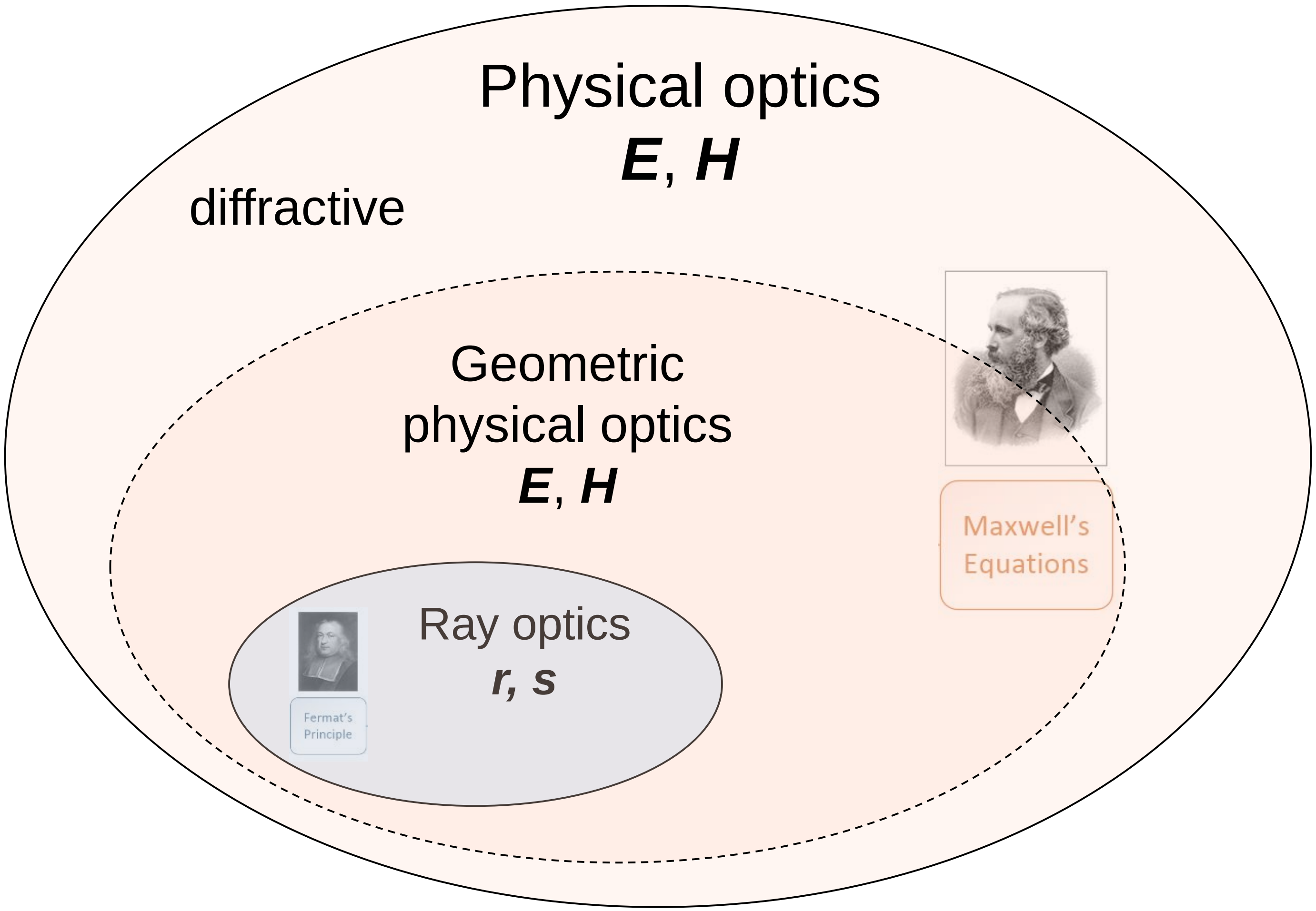
"According to traditional terminology, one understands by geometrical optics this approximate picture of energy propagation, using the concept of rays and wave-fronts. In other words polarization properties are excluded. The reason for this restriction is undoubtedly due to the fact that the simple laws of geometrical optics concerning rays and wave-fronts were known from experiments long before the electromagnetic theory of light was established. **It is, however, possible, and from our point of view quite natural, to extend the meaning of geometrical optics to embrace also certain geometrical laws relating to the propagation of the 'amplitude vectors' E and H."**

Geometric Field Equations

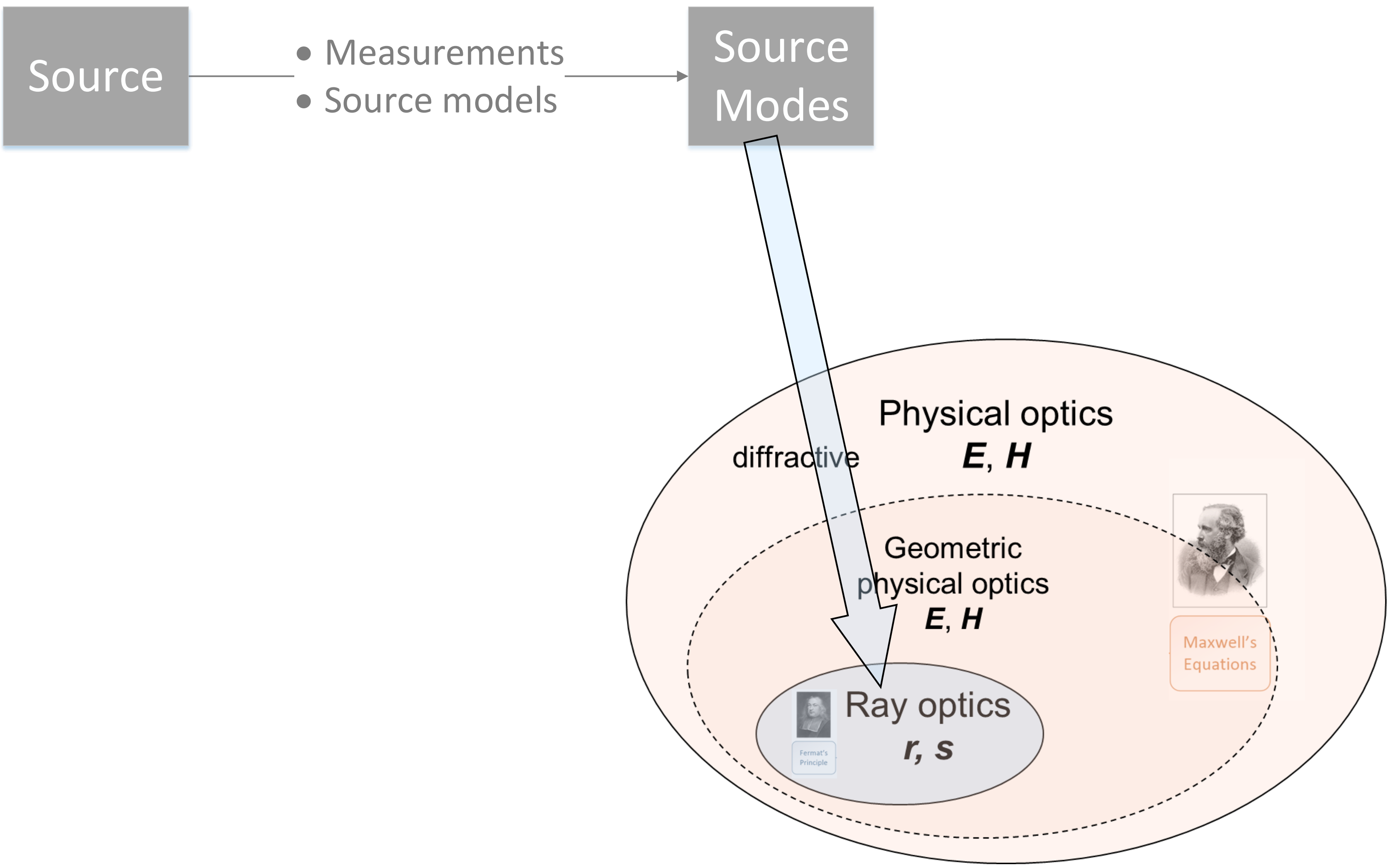
We follow Max Born's and
Emil Wolf's point of view!

Development and implementation of
algorithms to solve Maxwell's equations
in its **geometric field approximation**!

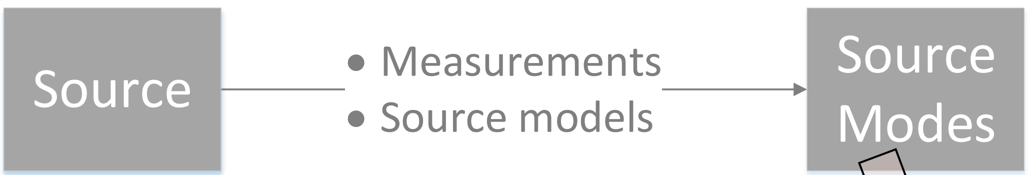
Ray and Field Tracing



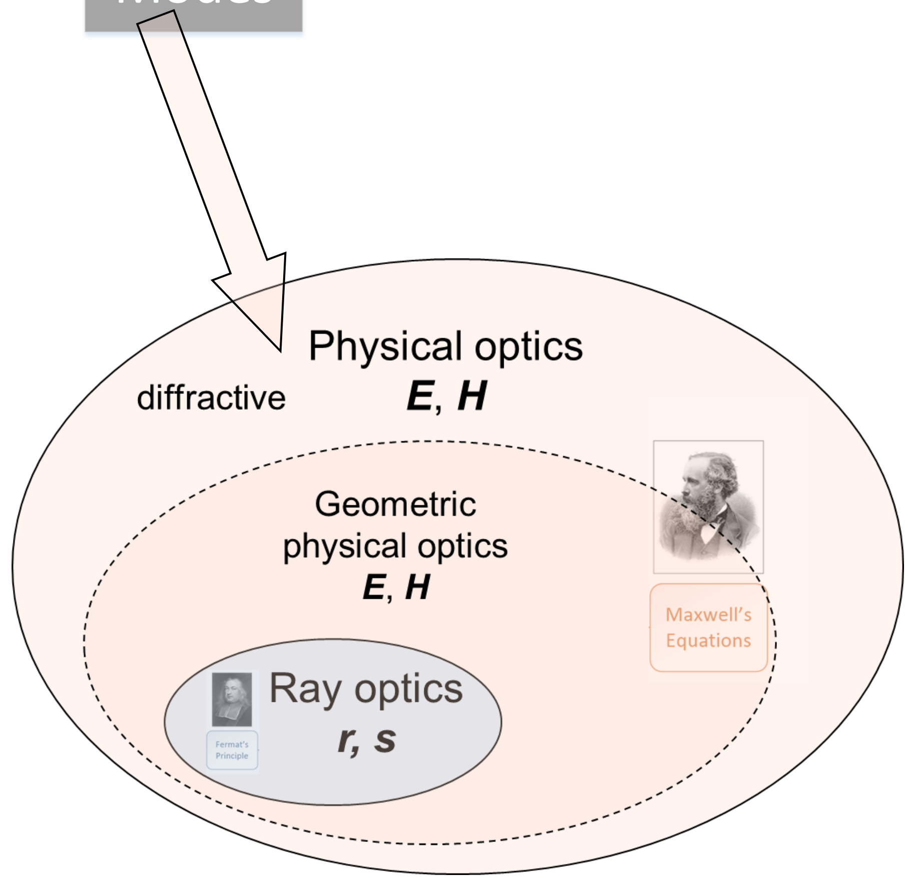
Source and System Modeling



Source and System Modeling

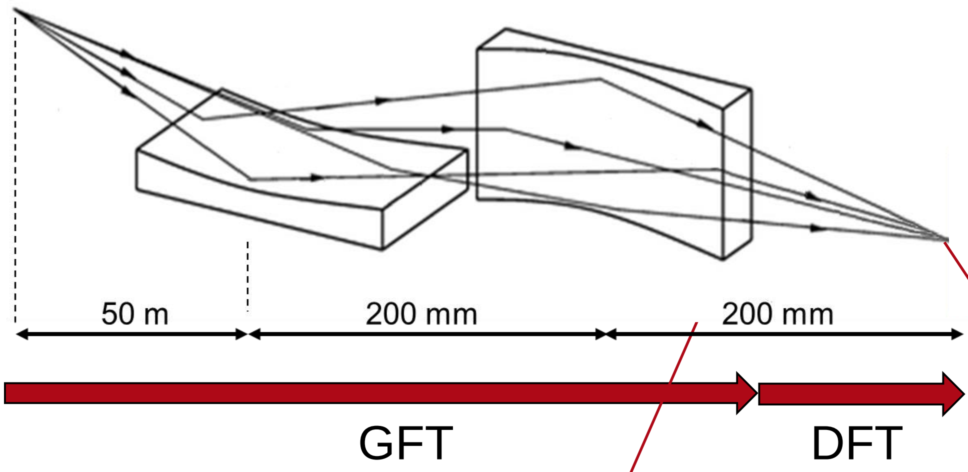


One of the hot topics and challenges in optical modeling and design in general!



System Modeling Example

Provided by Idir Mourad, BNL

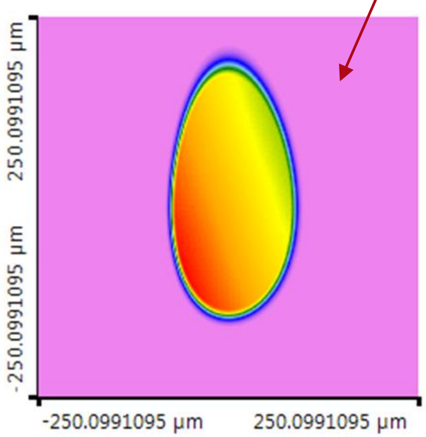


Source

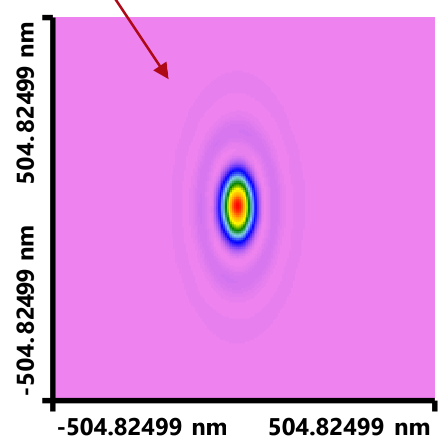
- **λ = 0.1 nm, 12 keV**
- Spherical wave, fully coherent field
- 50 m to mirror,12 μrad opening angle

Mirrors

- Elliptical, focal points at source & focal plane
- Gracing angle: $\theta = 3$ mrad

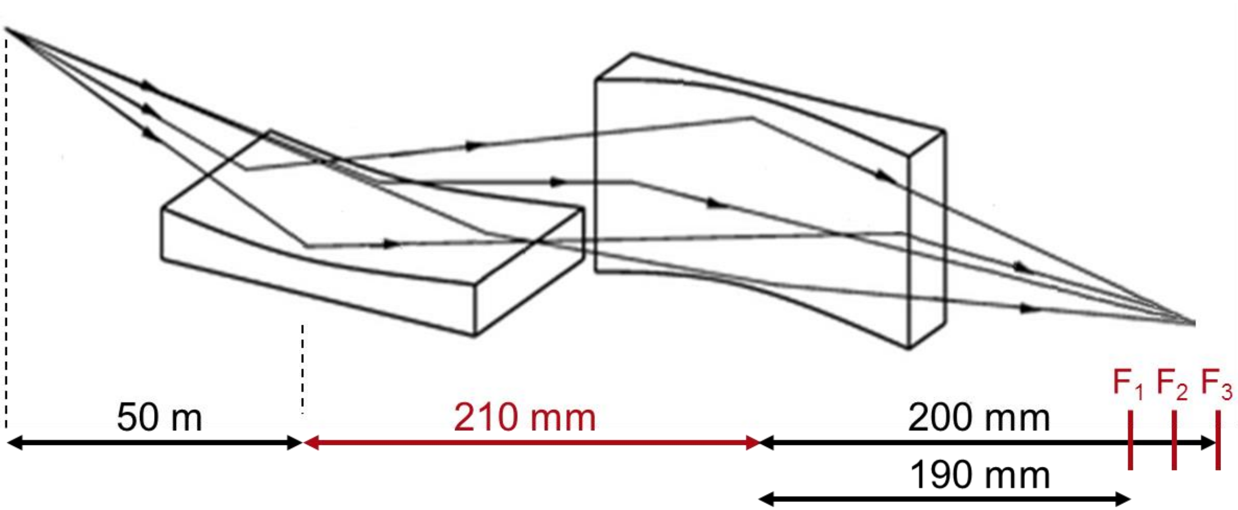


Field obtained by GFT behind the second mirror

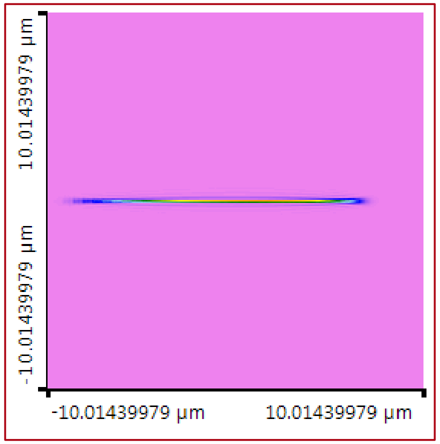


Field obtained by DFT in focal plane

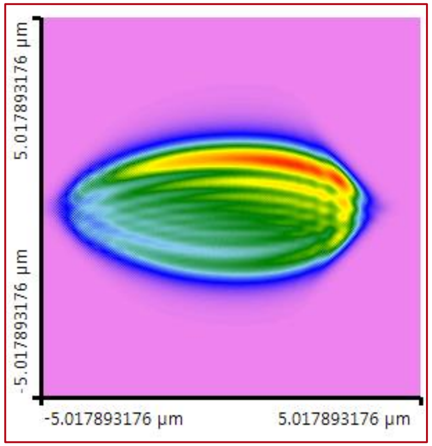
System Modeling Example: Tolerancing



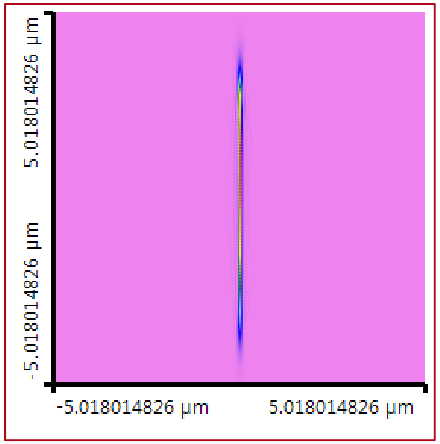
Field in F_1



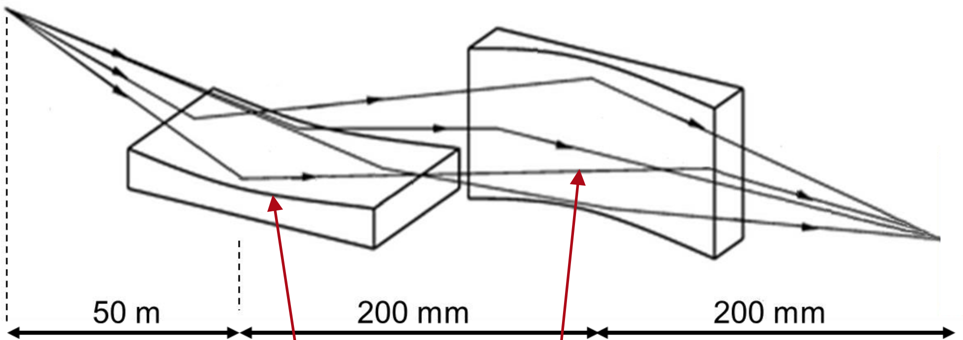
Field in F_2

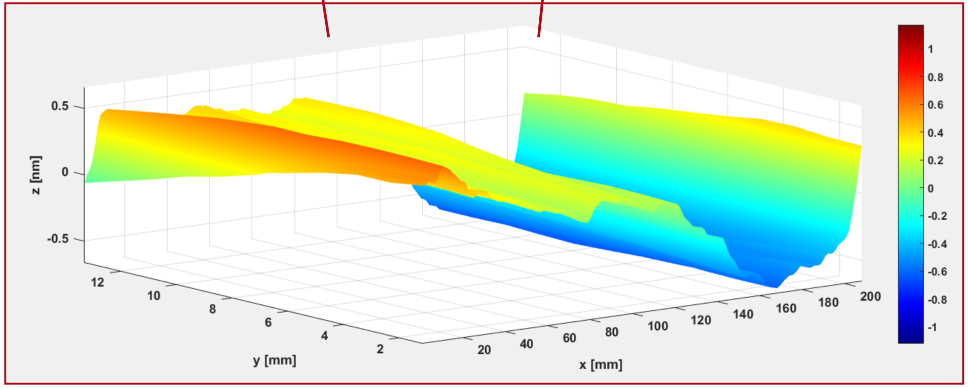


Field in F_3



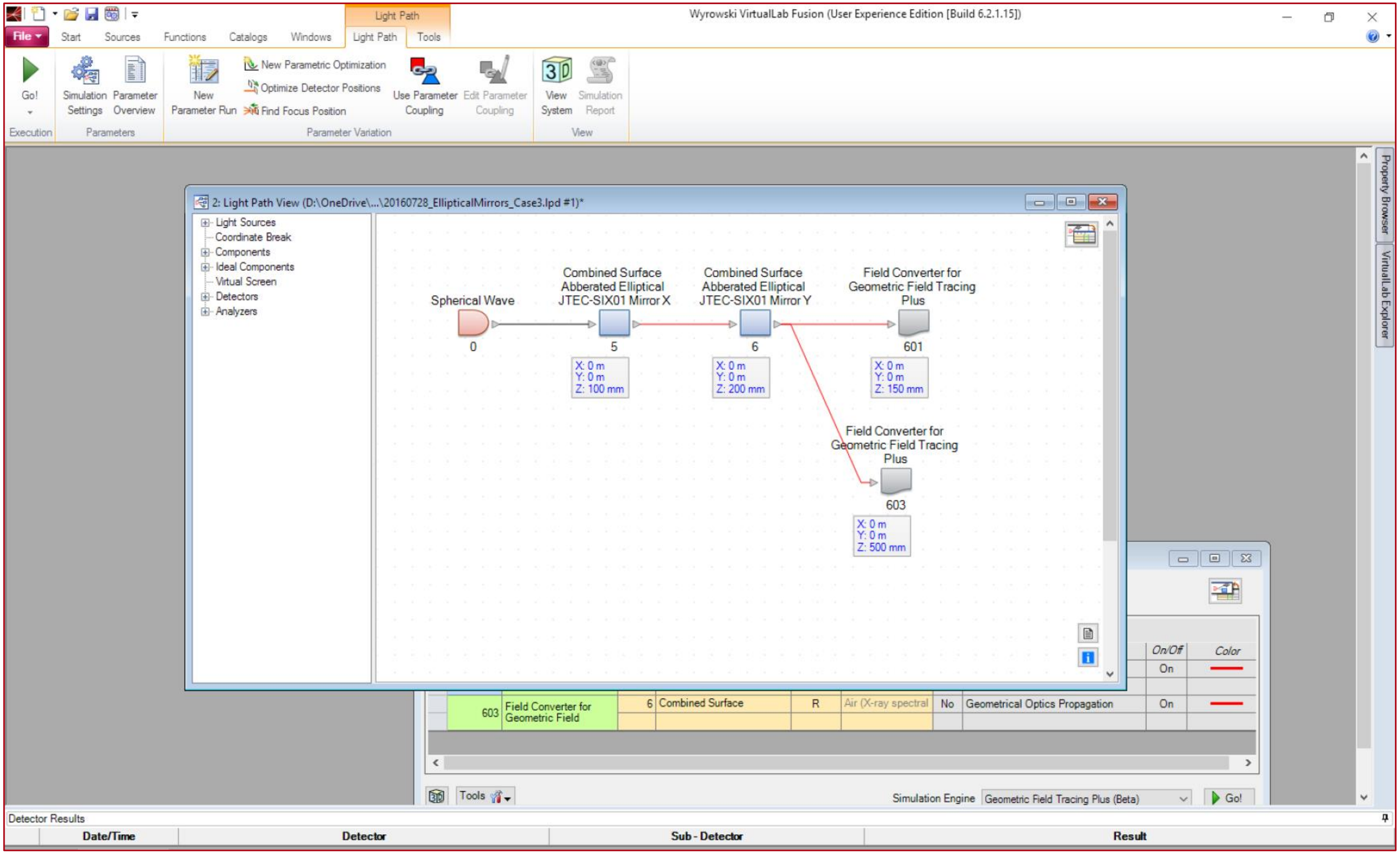
System Modeling Example: Tolerancing



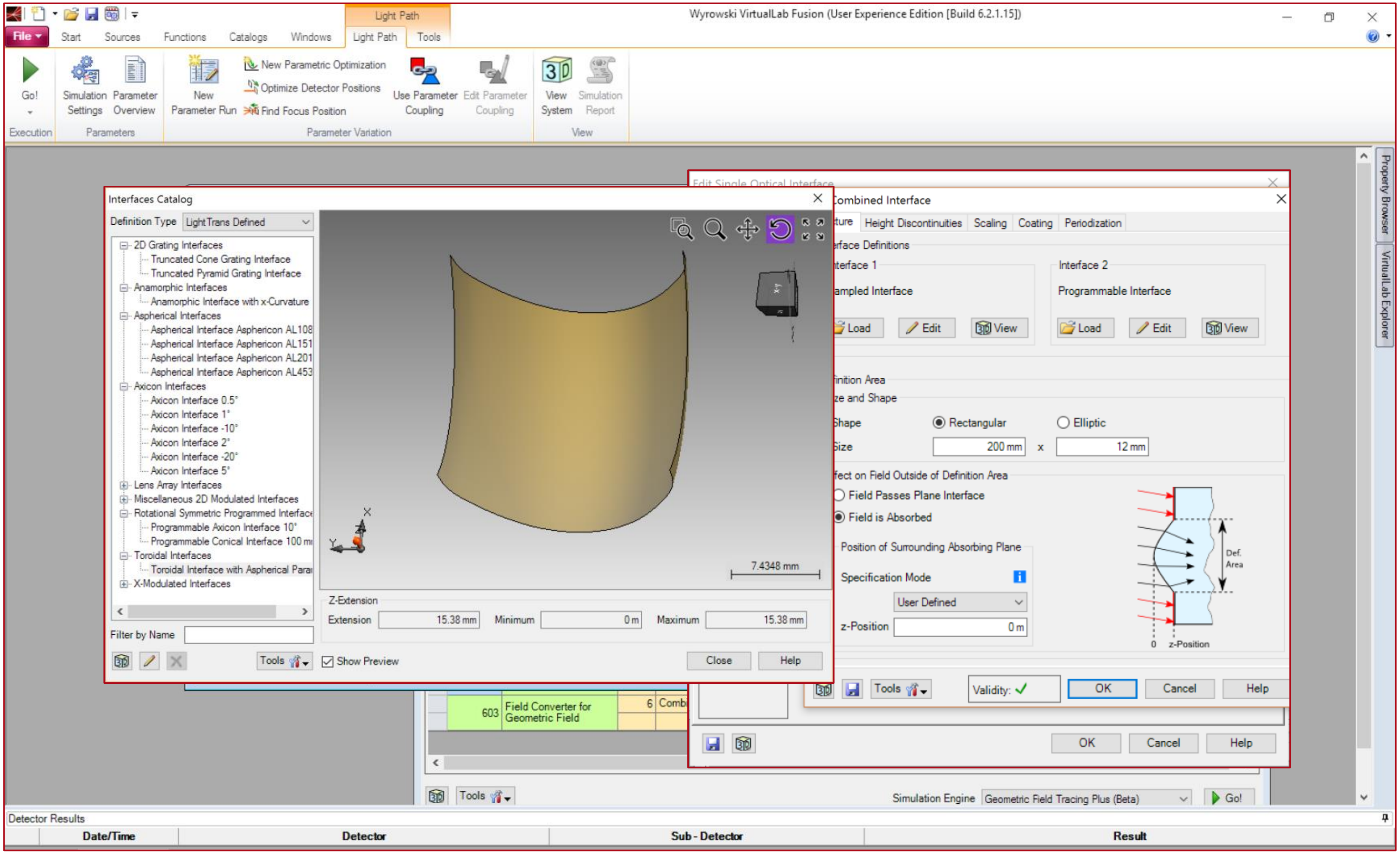


Measured error map, PV ~ 1.2 nm
provided by Idir Mourad, BNL

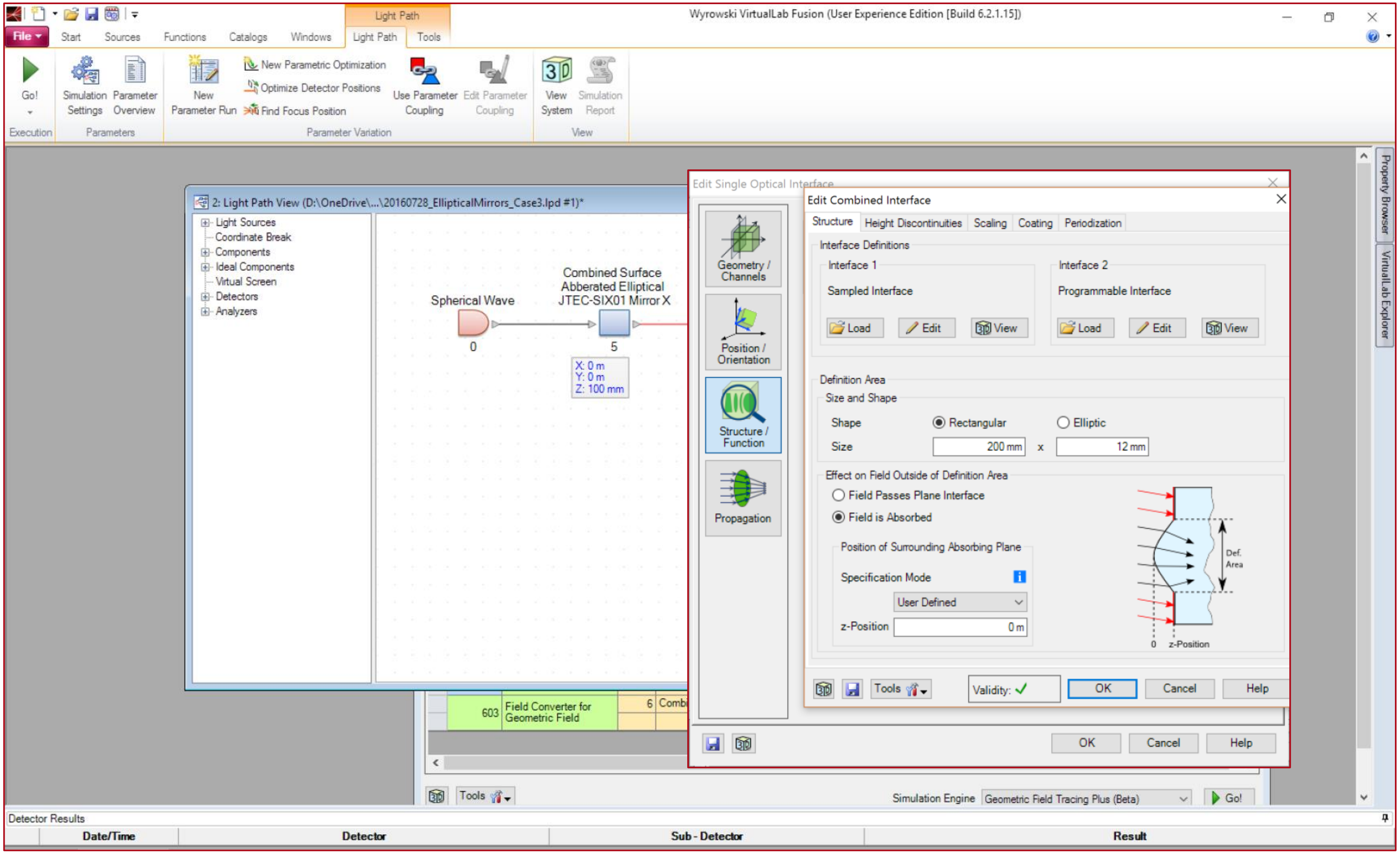
System Modeling Example: Tolerancing



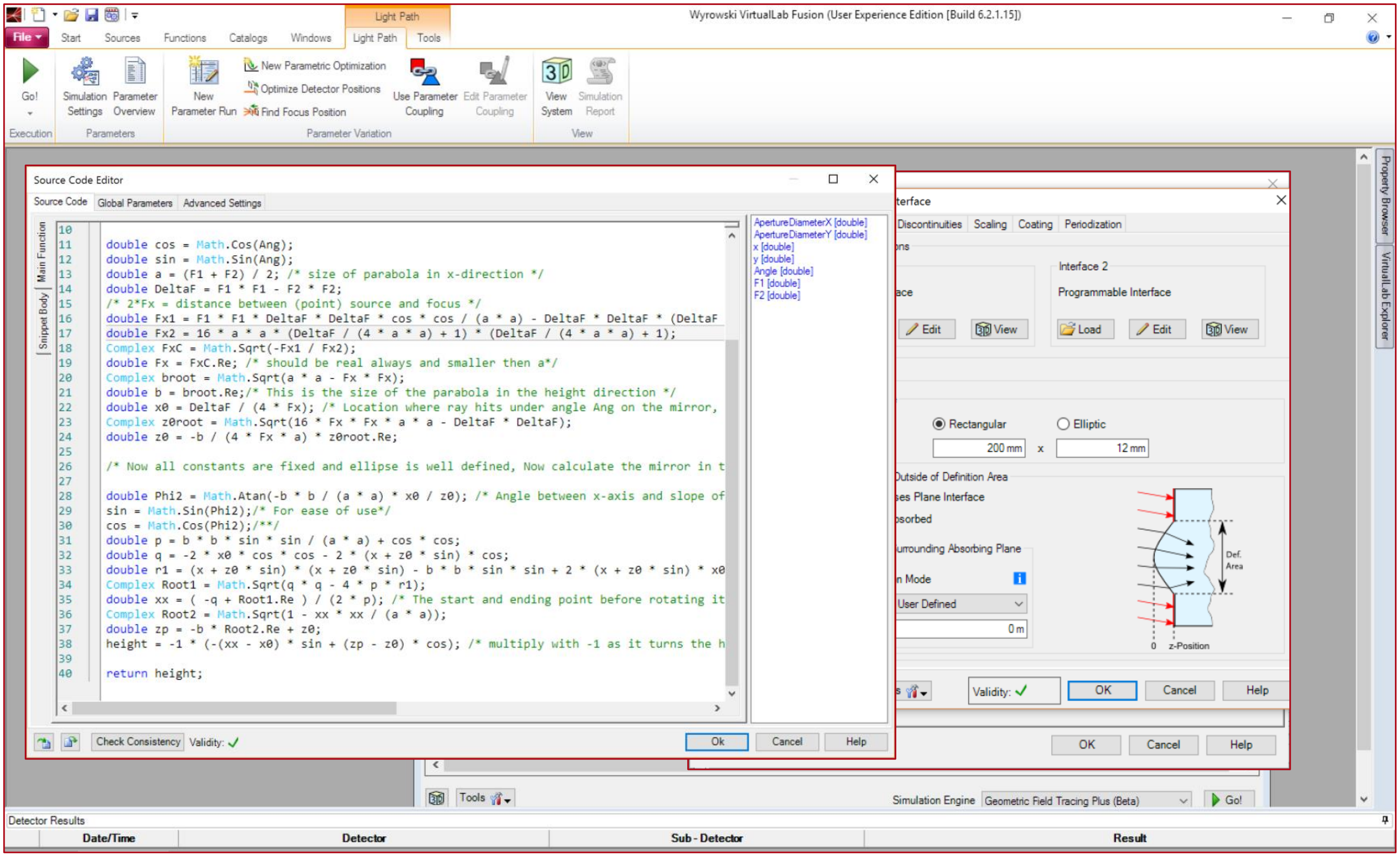
System Modeling Example: Tolerancing



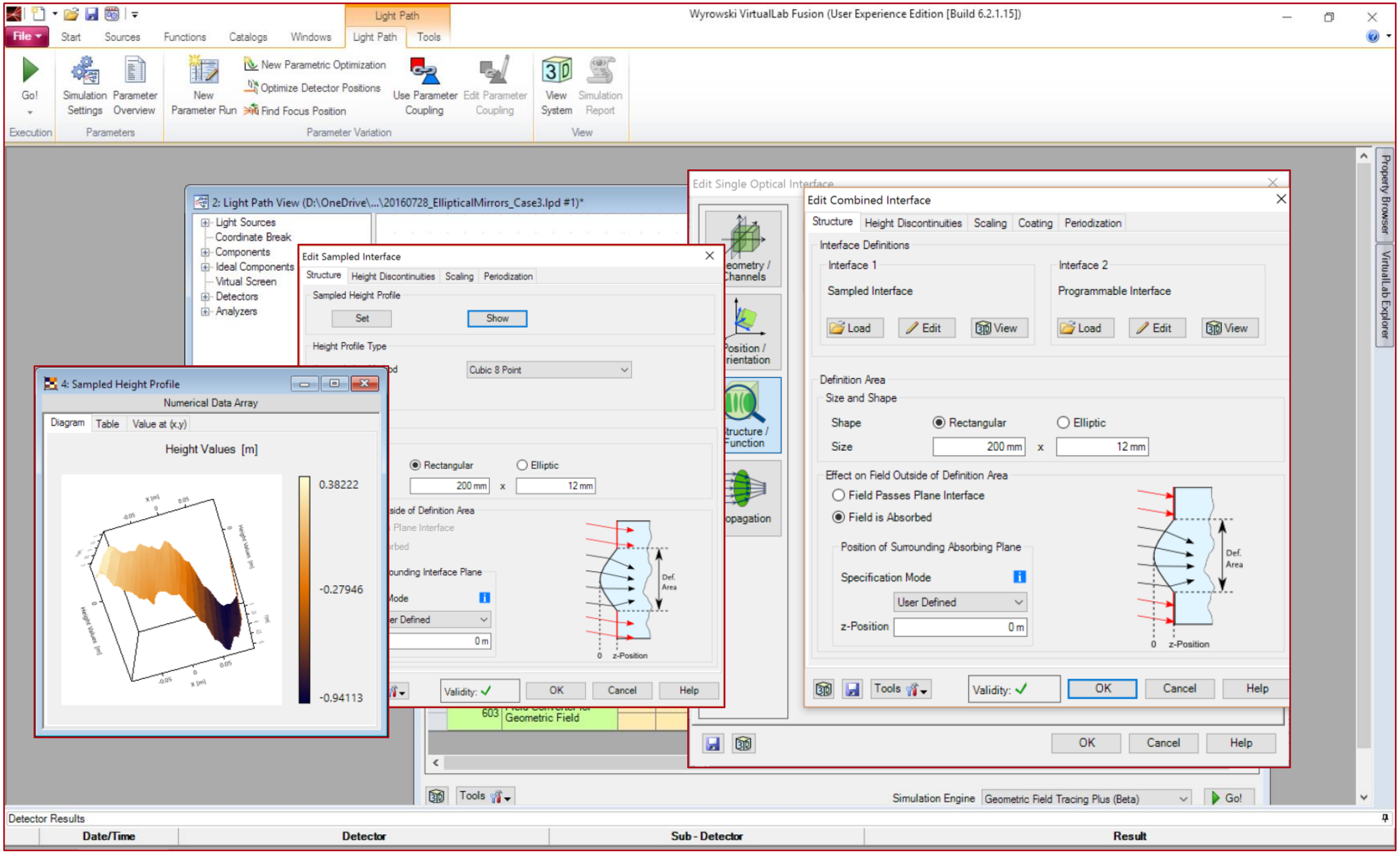
System Modeling Example: Tolerancing



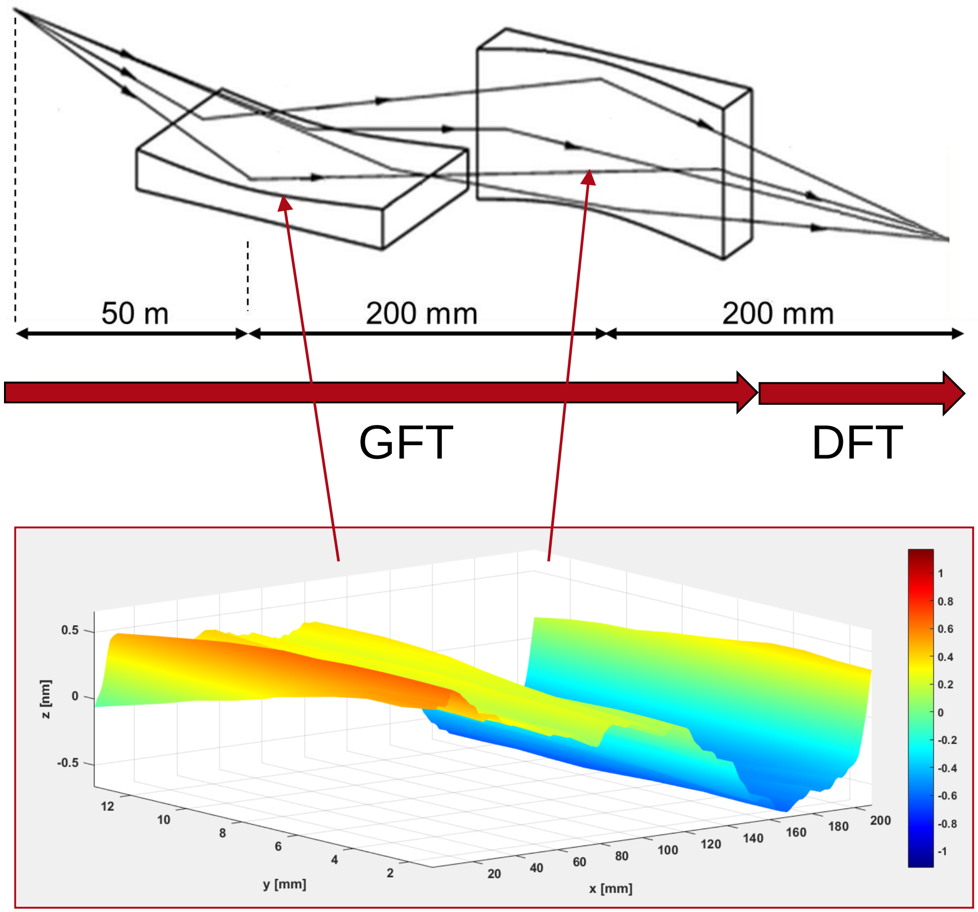
System Modeling Example: Tolerancing



System Modeling Example: Tolerancing



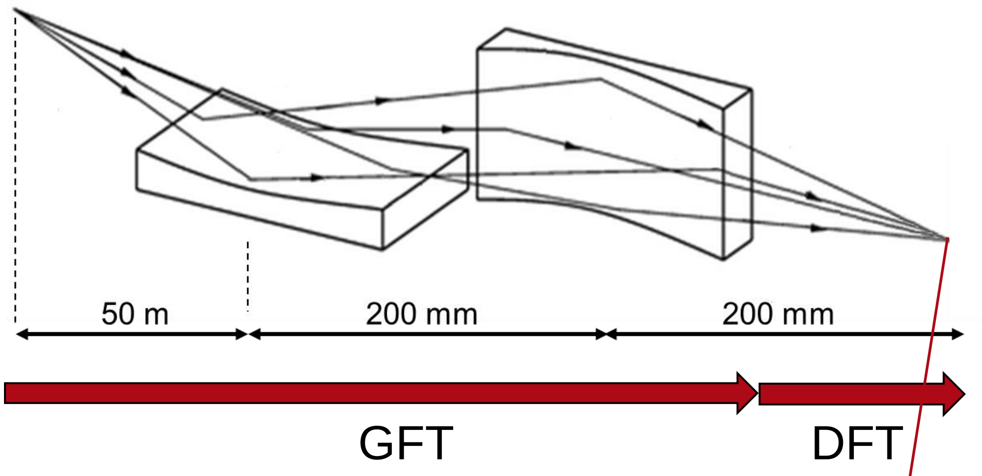
System Modeling Example: Tolerancing

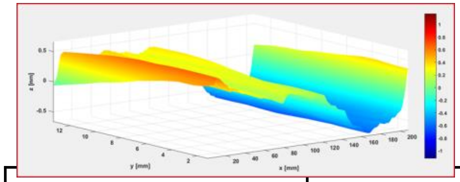


Measured error map, PV ~ 1.2 nm
provided by Idir Mourad, BNL

Case	Strehl Ratio
Ideal	1.0000
1x Errormap	0.9933
5x …	0.9445
10x …	0.7903
20x …	0.3964

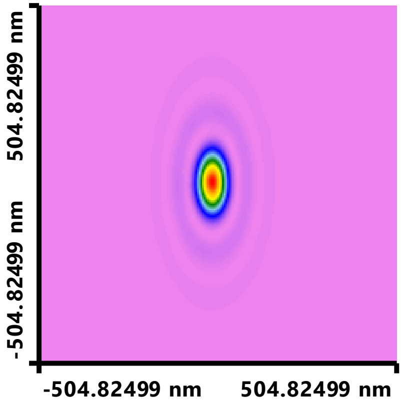
System Modeling Example: Tolerancing



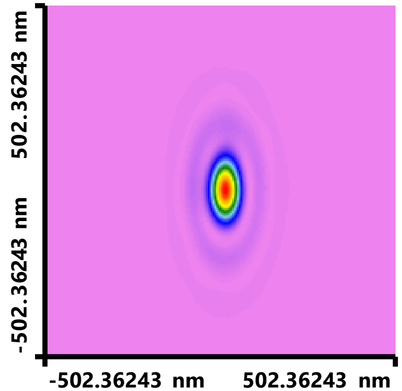


Case	Strehl Ratio
Ideal	1.0000
1x Errormap	0.9933
5x …	0.9445
10x …	0.7903
20x …	0.3964

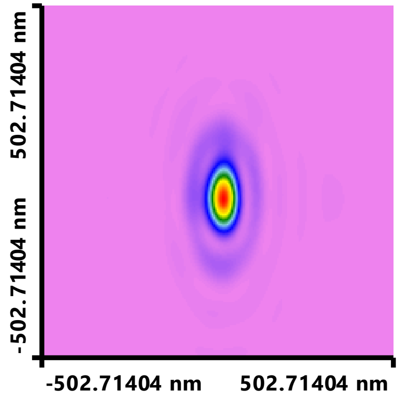
Error map (1x)
FWHM: 61 x 126 nm



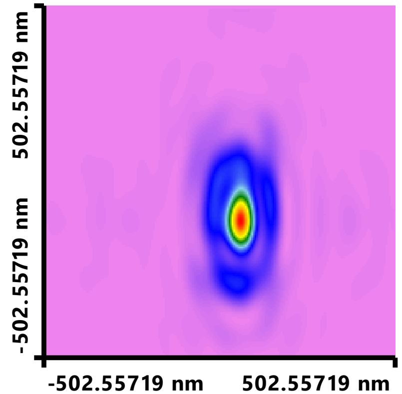
Error map (5x)
FWHM: 62 x 127 um



Error map (10x)
FWHM: 63 x 128 um



Error map (20x)
FWHM: 62 x 130 um



VirtualLab Fusion is a fast physical optics modeling and design software.

Could be powerful tool for x-ray modeling!

We encourage you to contact us to find out, how good we can treat with your modeling and design tasks.

Common paper as result would be fine!