Overview of Direct Geometry Spectroscopy

IKON5

Lund, 2013-09-25 & 26

EUROPEAN SPALLATION SOURCE

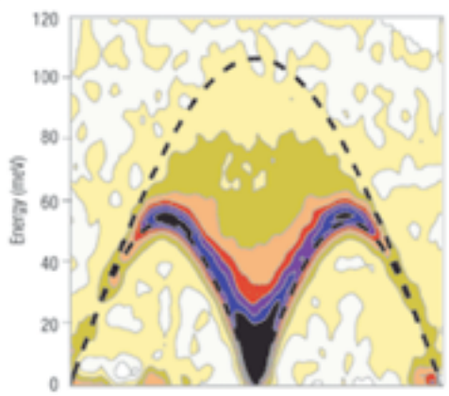
P. P. Deen

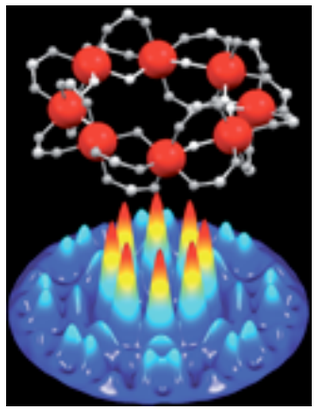
Chopper spectroscopy

Direct Geometry Spectroscopy (DGS)

Diverse Science Drivers:

Magnetism
Superconductivity
Functional materials
Gas storage materials
Soft matter
Life sciences.





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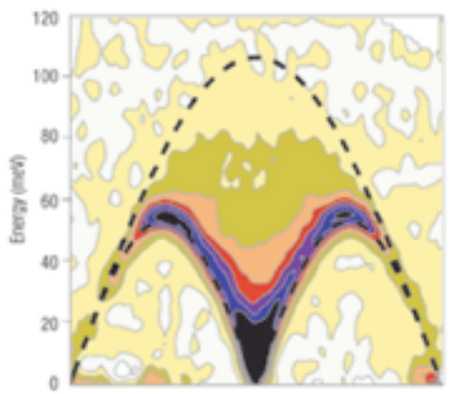

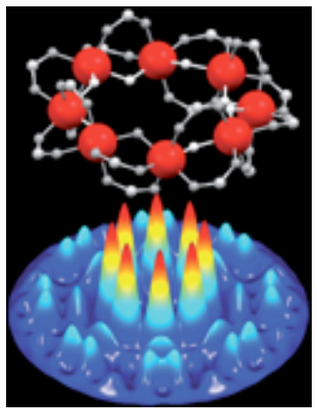

Diverse Science Drivers:

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Superconductivity
Functional materials
Gas storage materials
Soft matter
Life sciences.

Wishes of the community:

More flux on sample.
Smaller samples areas.
Parametric studies. Kinetics/in-operando
Simultaneous application of extreme conditions.
Cover as much 'time' range without compromising intensity.

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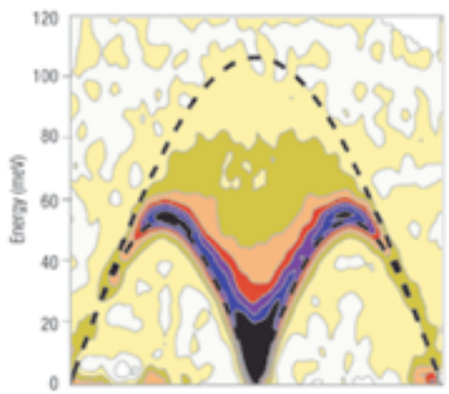

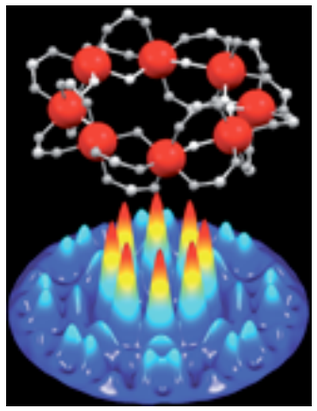

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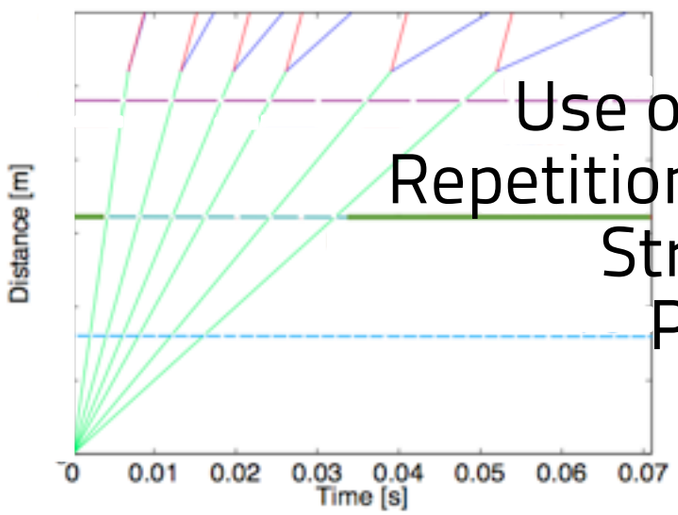

Technical :

Use of 2.86 mS (broad vrs narrow bandwidth).
Repetition Rate Multiplication: Novel chopper designs.
Strong emphasis placed on background.
Polarisation Analysis or future proof.
Detectors.

DGS: Instrument Work Units

- **Cold chopper spectrometer (German WU - TUM) (2013)**
  - is dedicated to studies of single crystal magnetism and soft matter. The narrow bandwidth instrument will provide an intense cold neutron beam with high-energy (1-3 %) resolution.

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- **High resolution thermal chopper spectrometer.(2014)**
  - optimized for high temperature superconductivity, multiferroics, low-dimensional magnetism, functional and hydrogenous materials.

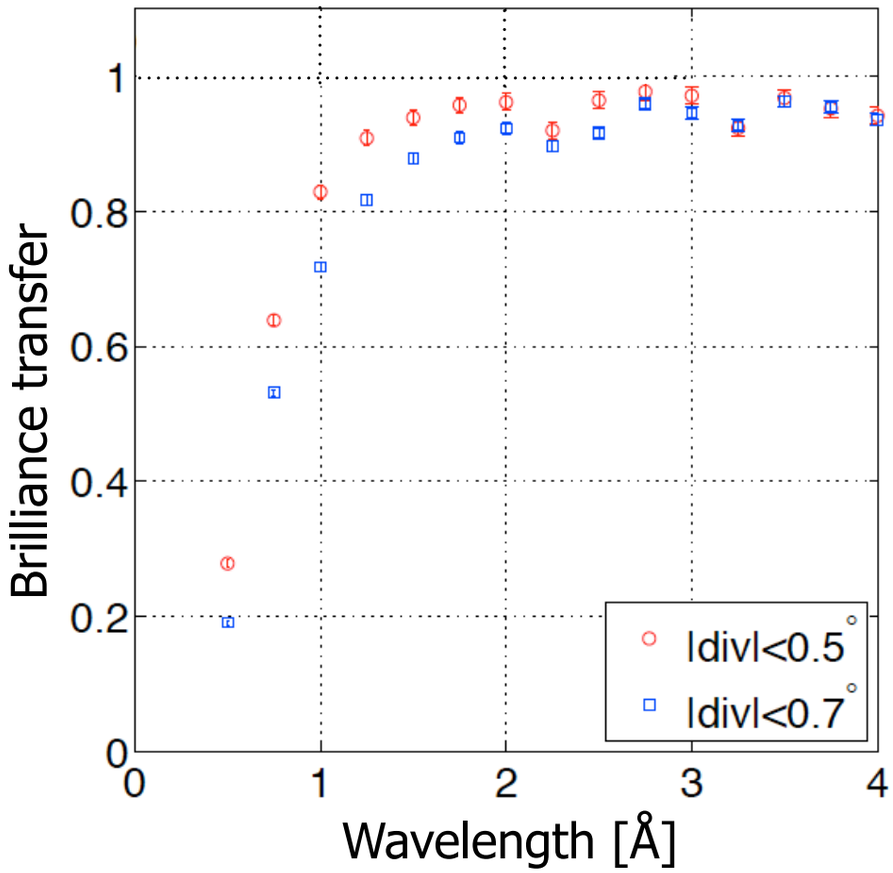
High resolution thermal chopper spectrometer

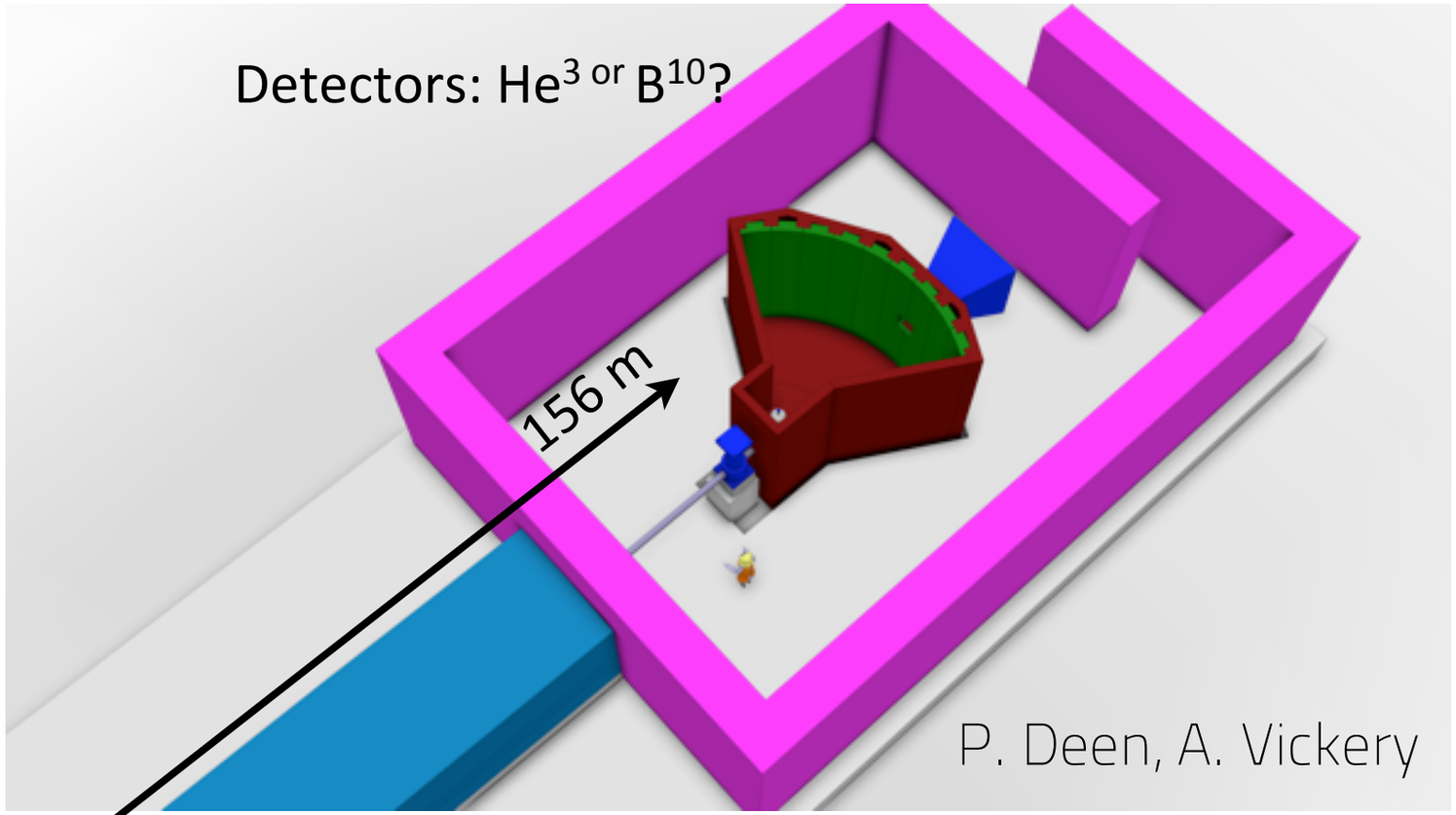
P. P. Deen & A. Vickery

Optimized for high temperature superconductivity, multiferroics, and low-dimensional magnetism, catalysis & gas storage

The instrument will simultaneously measure 11 < E_i < 167 meV (300 meV) and will be optimized for ΔE /E = 2 % with tighter energy resolutions possible.

Guide Length:156 m





Thank you!

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P. P. Deen

Chopper Spectroscopy

VOR
Versatile Optimal Resolution chopper spectrometer

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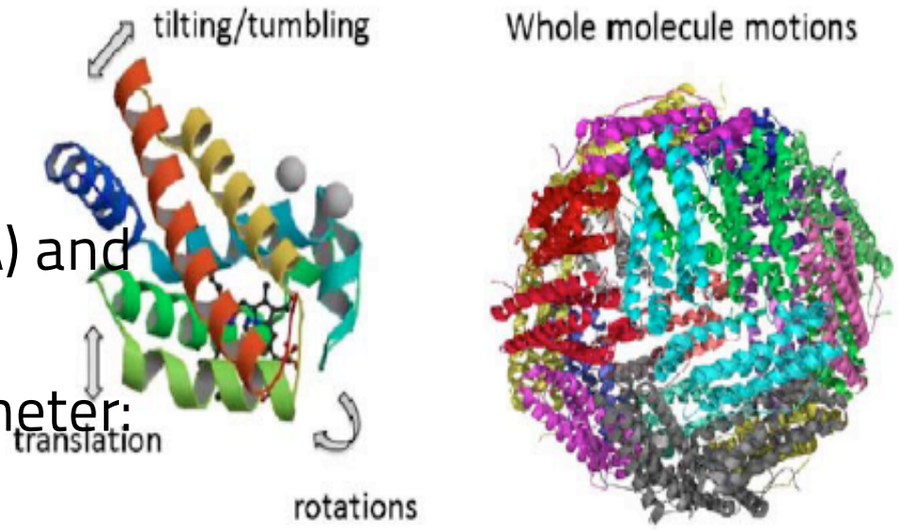
VOR
Goddess who knows all

Pascale P. Deen
Anette Vickery

IKON 25 - 26th September

Science case I



Soft matter: multi-scale with ξ(spatial) (typically 10 - 1000 Å) and ξ(timescales) (10-^{12} up 10^{4} seconds)

Use backscattering/ cold/thermal INS/ vibrational spectrometer:
Inhomologous samples
Time-limited samples
Difficulties with data analysis

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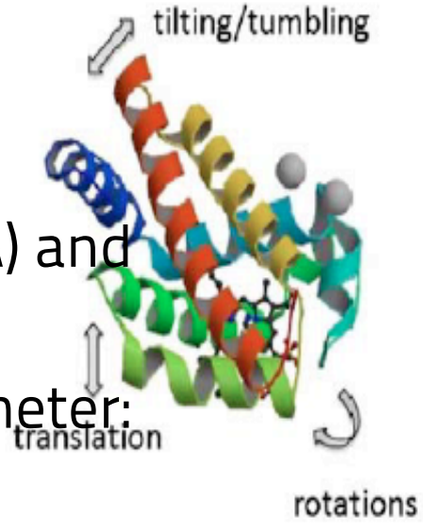

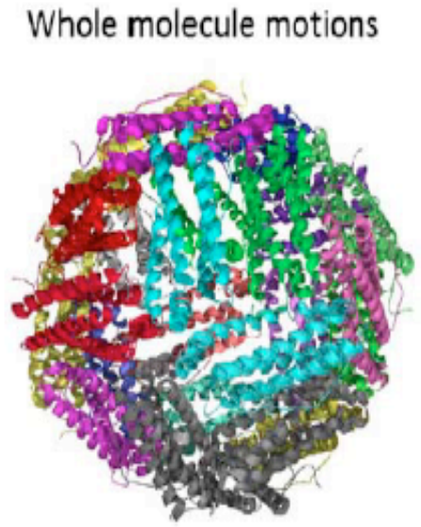

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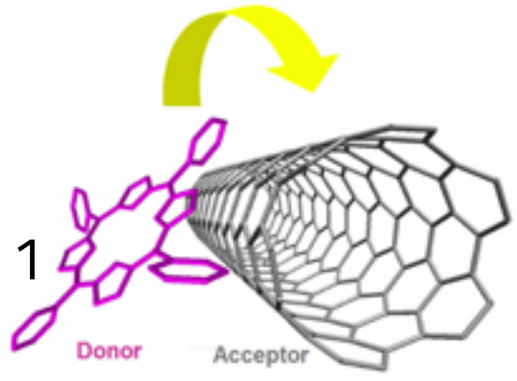
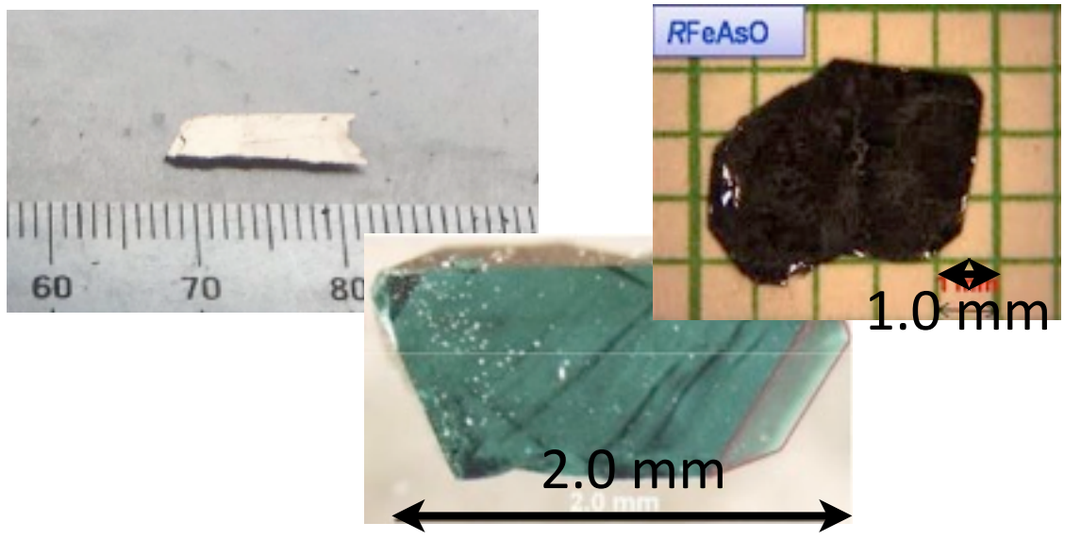
Functional Materials: Current limit is flux. The community would like to probe phase space (Pressure - 0 < P < 9 GPa) - need samples as small as 1 mg (currently 500 mg is feasible).
Dynamic range: QES, external modes (0-10meV), radial modes(30 - 100 meV), tangential modes (100 - 200 meV).

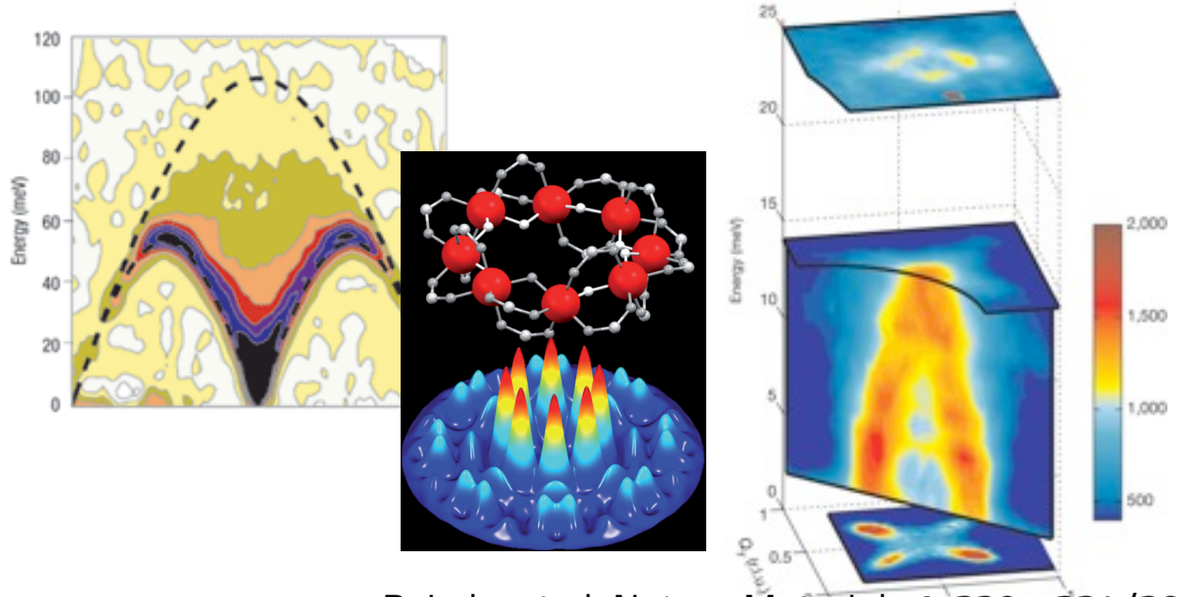


Laboratoire Pierre Aigrain.

Science case II

Magnetism and superconductivity: Novel compounds difficult to synthesise - small.
Need to perturb ground states (simultaneous H, P) - limited sample sizes. Require excellent S/N
Quantum effects: Weak cross sections with broad continua. Broad dynamic range benefit from simultaneous fits of data to models across all the dynamic features.





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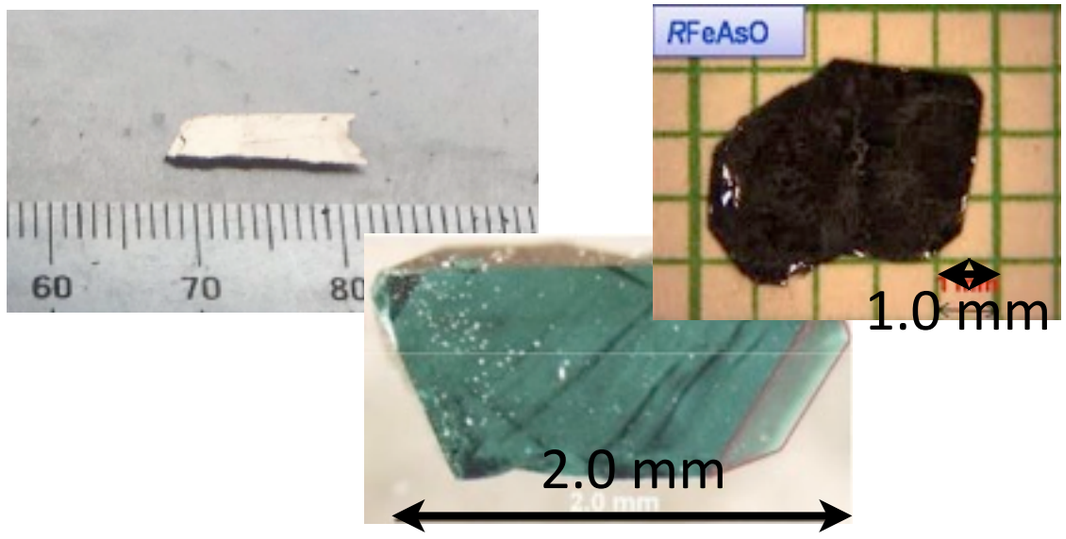

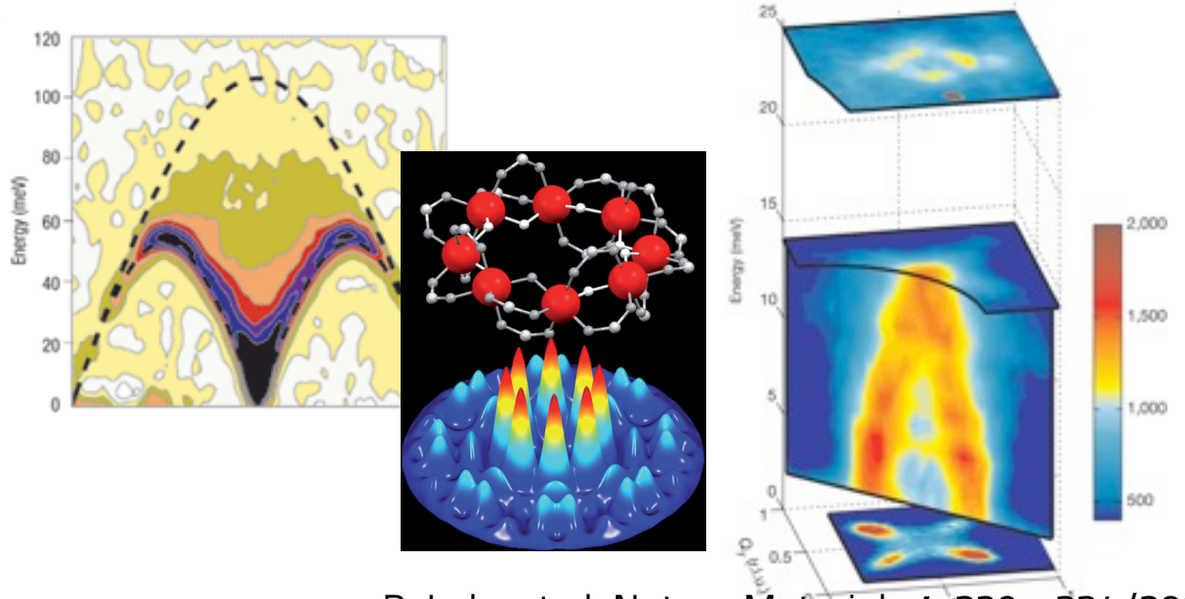

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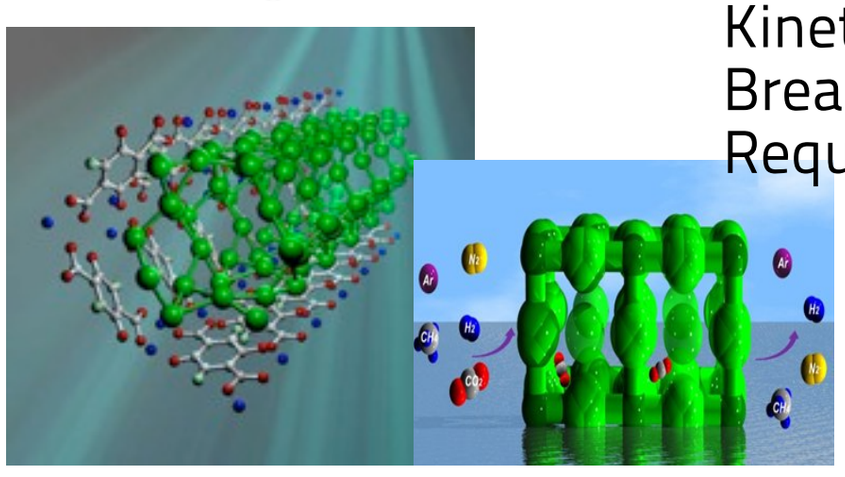
Gas storage and catalysis: Limited number of studies (flux limit)
Kinetics: second - hour timeframe/in operando.
Breakthrough for inelastic measurements on a second timeframe.
Requires two orders of magnitude in flux.



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Neil Champness, University of Nottingham

What do we need to deliver

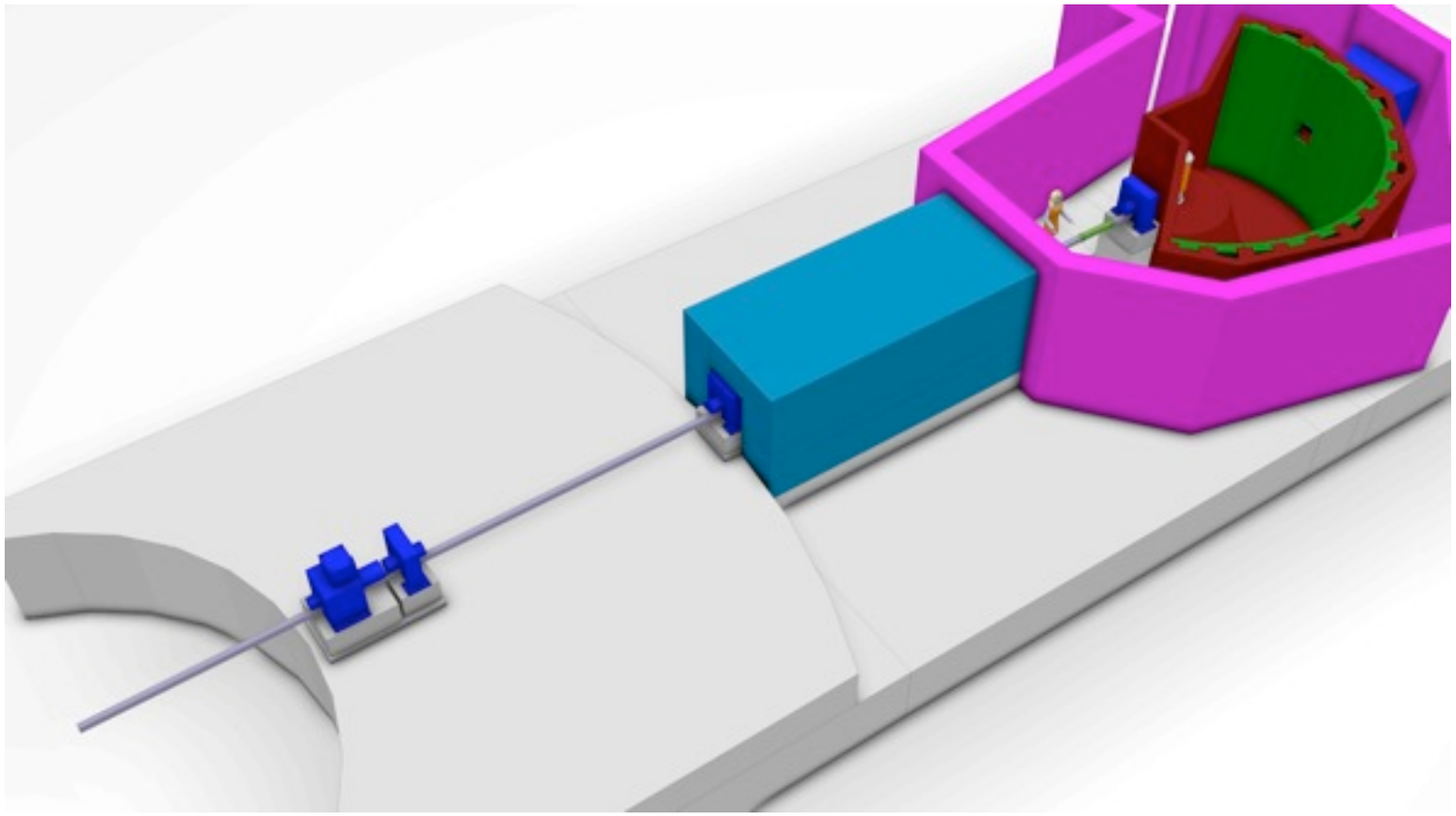
Soft matter: Broad bandwidth
Variable energy resolution (several μeV - 3000 μeV)
Be able to relax resolution for weak scattering signals
Availability of high momentum transfer (Q < 11 Angstrom)
High flux but not necessarily point like.
Currently limited number of Q dependent studies but future ….

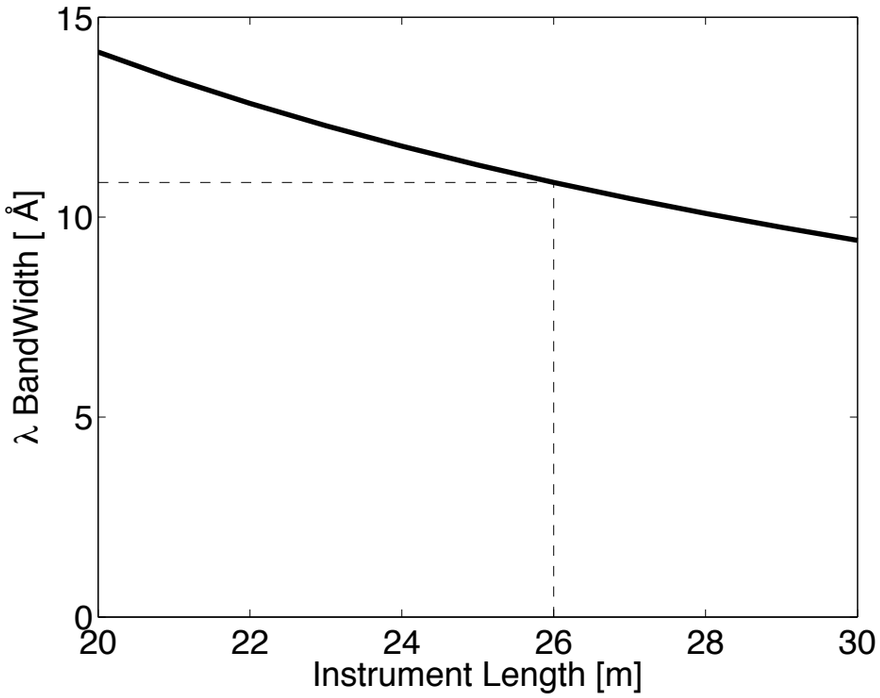
Functional materials: Broad bandwidth (0 - 200 meV),
Clean/limited and flat flux profiles (but not too small)
High flux (x 10 - 100) probe (P) phase space.
High resolution at high energies.

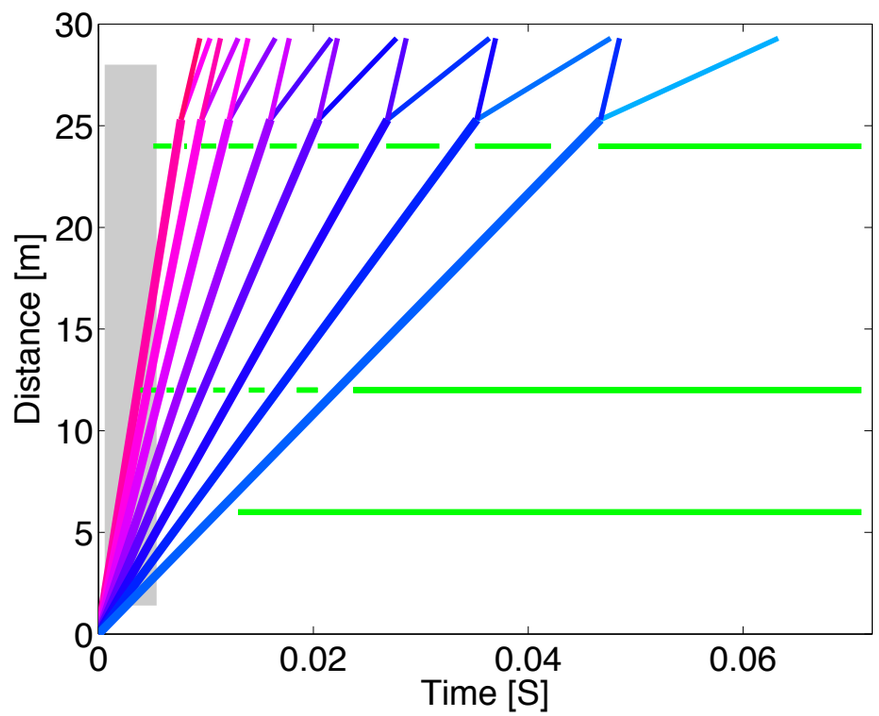
Magnetism: Broad bandwidth (some)
Flux focussed on small samples.
Q-dependence important, clean divergence profiles
High energy resolution - ΔE/E ~ 1-3%

Gas Storage & Catalysis: Broad bandwidth
In-operando studies (second)
Small samples but not point like.
Two orders of magnitude in flux

VOR - Wide bandwidth bispectral chopper spectrometer
Versatile Optimal Resolution chopper spectrometer







Main parameters (Optimisation = wishes/reality):
Moderator to sample = 26 m ΔE ~ 10 Å.
Bispectral extraction: rotation.
Measure in the first time frame using RRM.
Prompt pulse does not fall into the data set.

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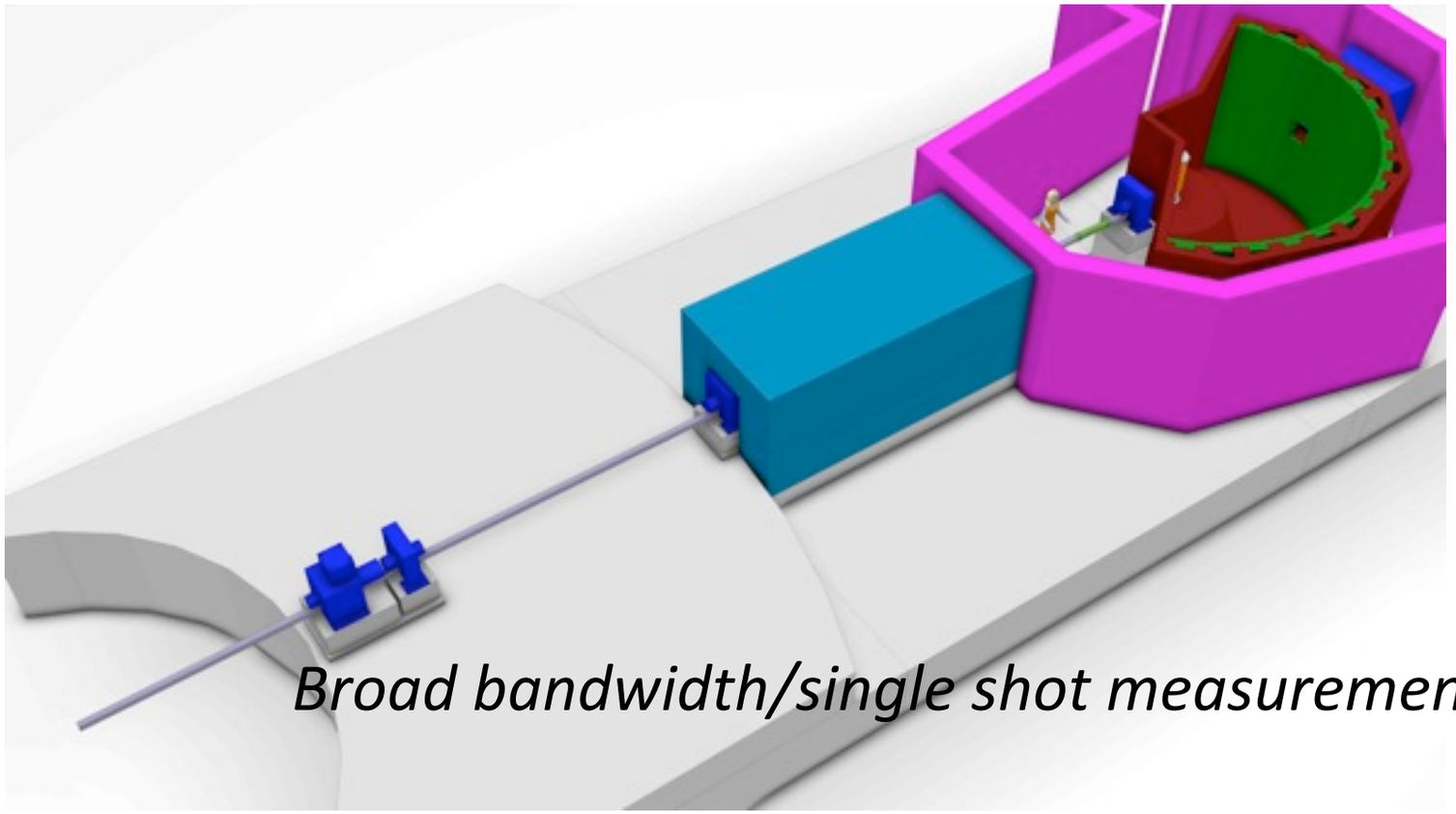
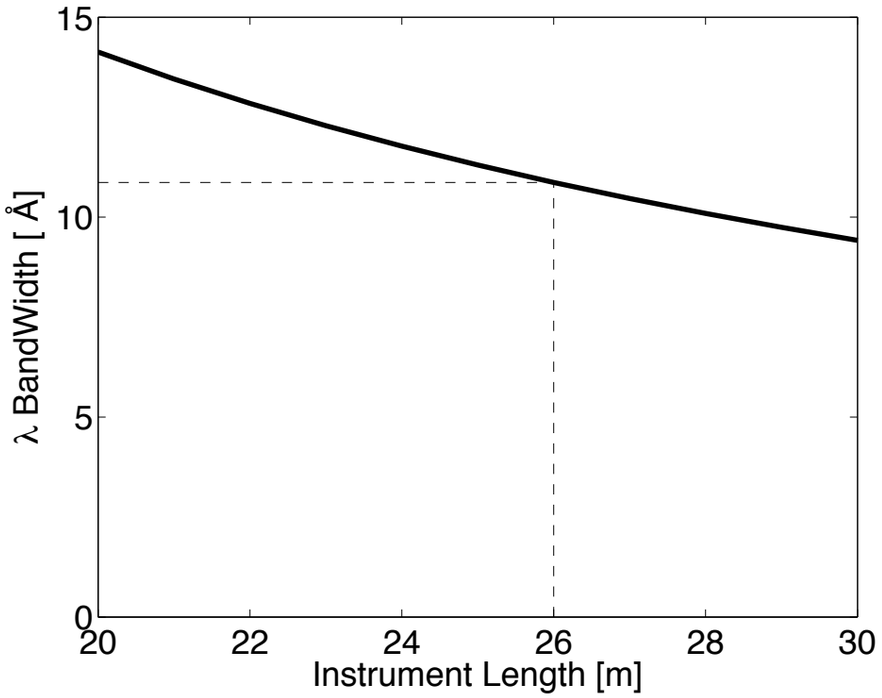
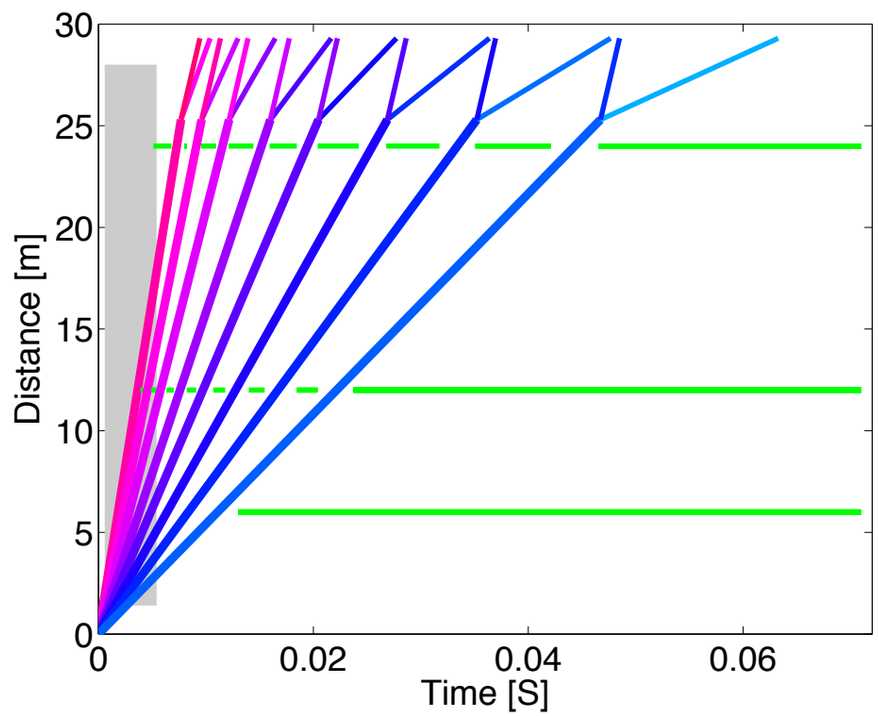




Broad bandwidth/single shot measurement of all excitations



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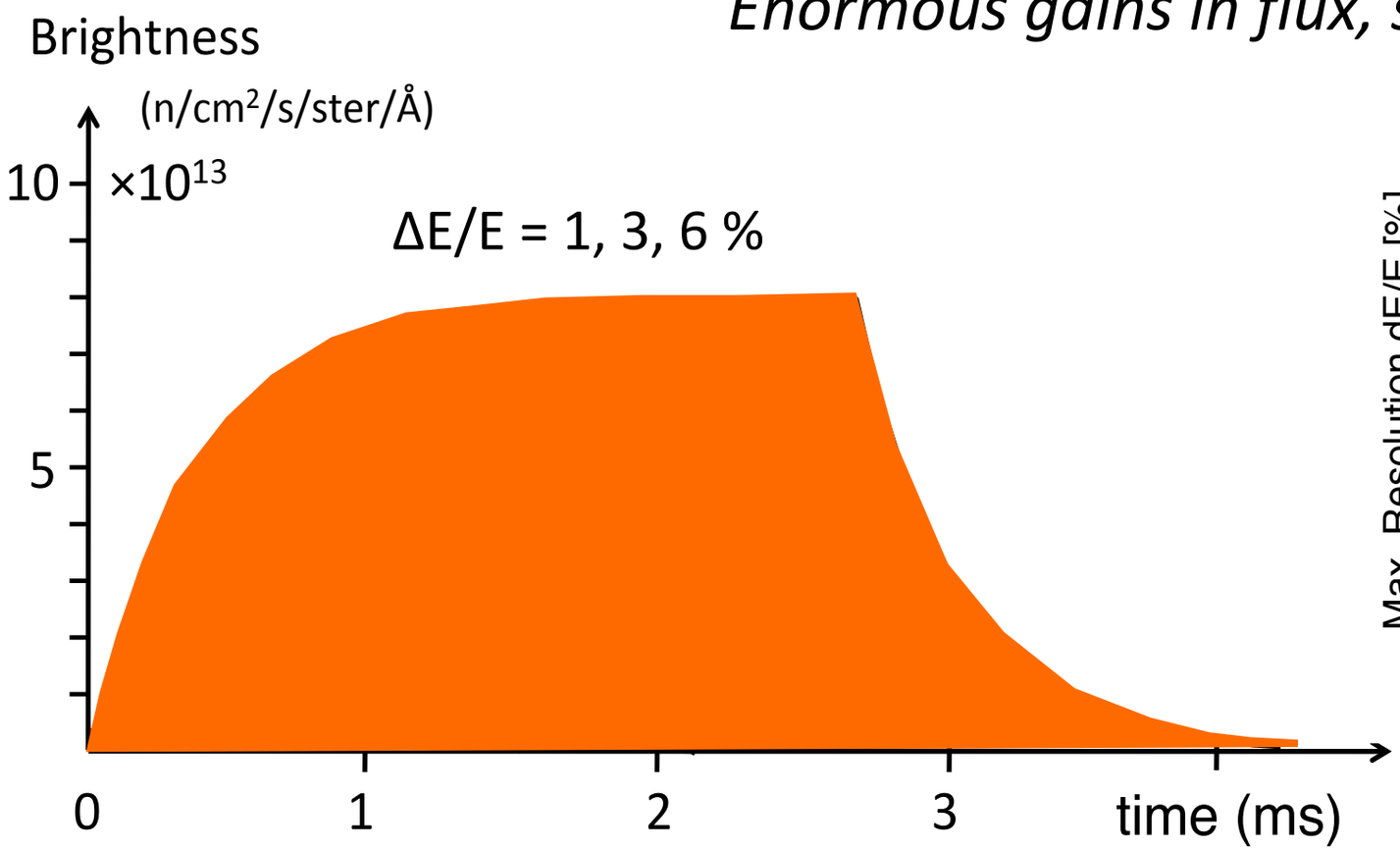
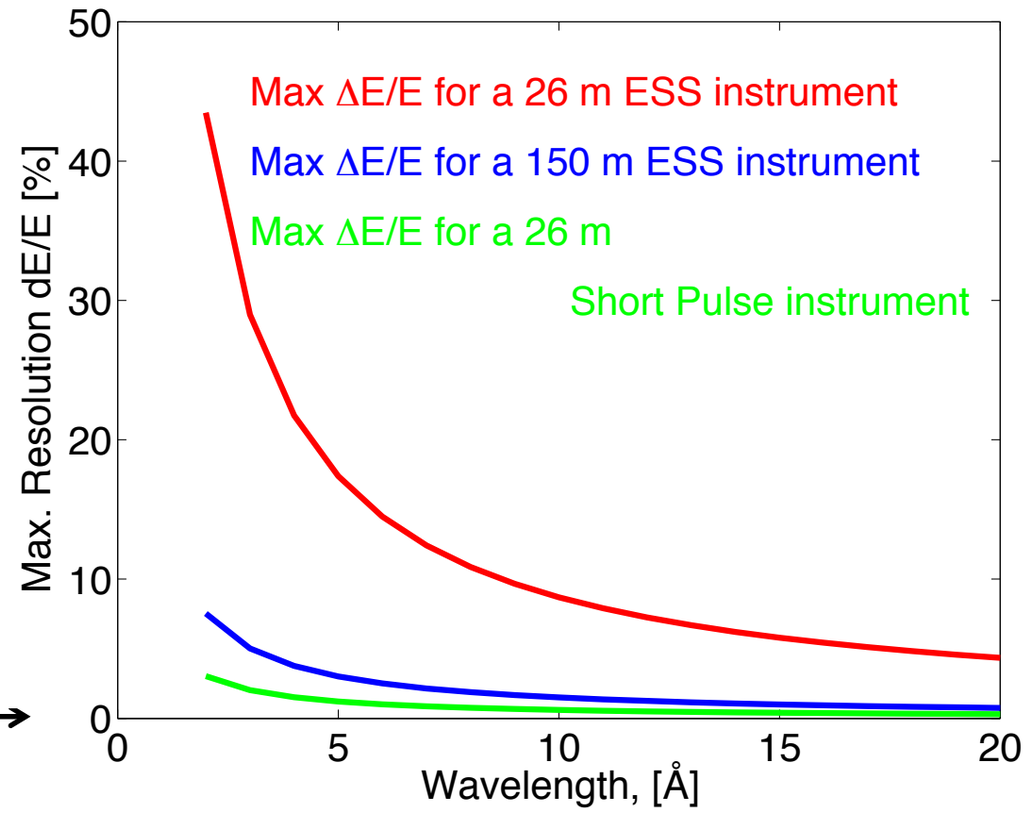
Energy resolution
Broad bandwidth & Trading flux for resolution

Enormous gains in flux, see later





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Max. resolution at large λ (pulse only) = ΔE/E = 6 %

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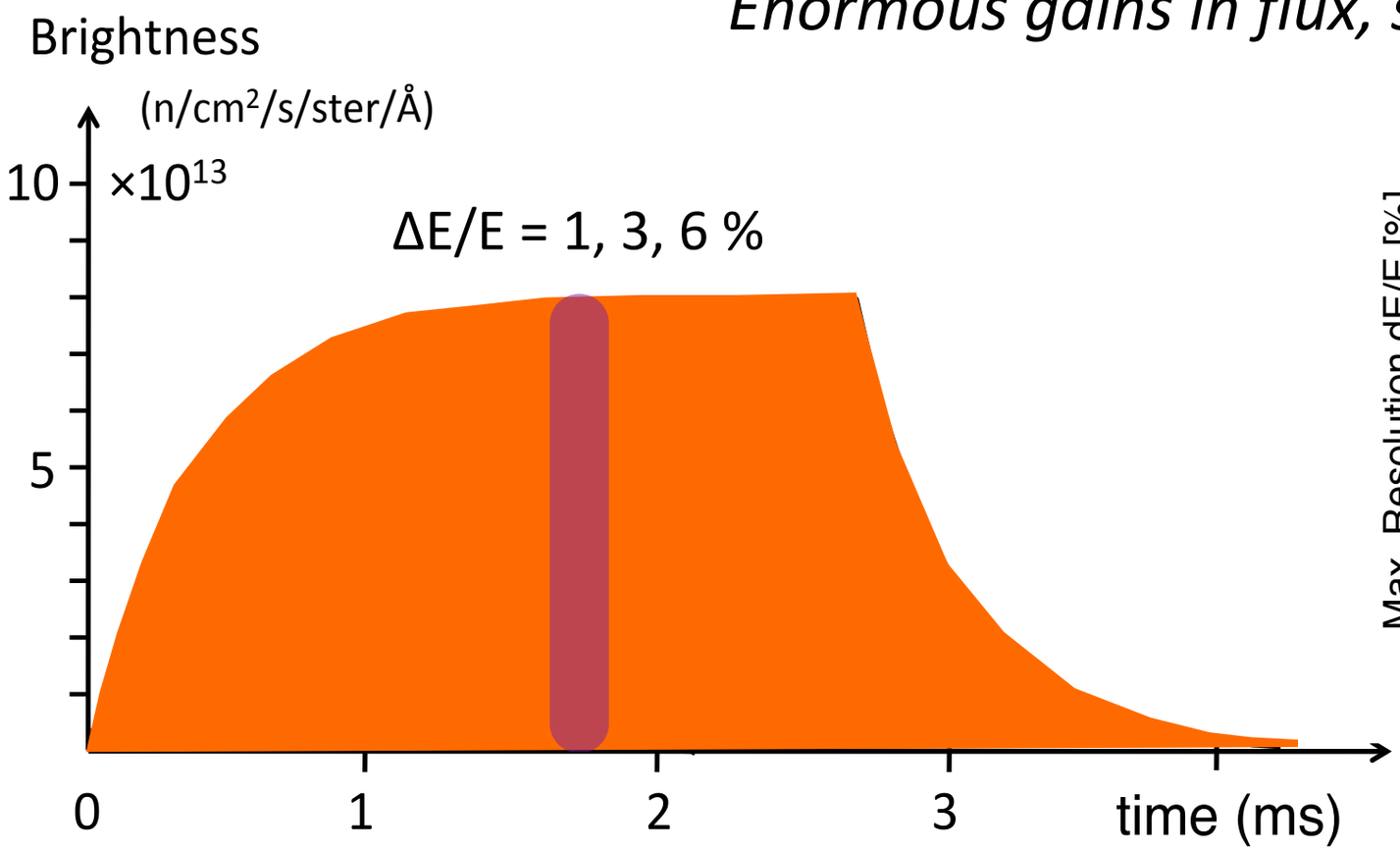

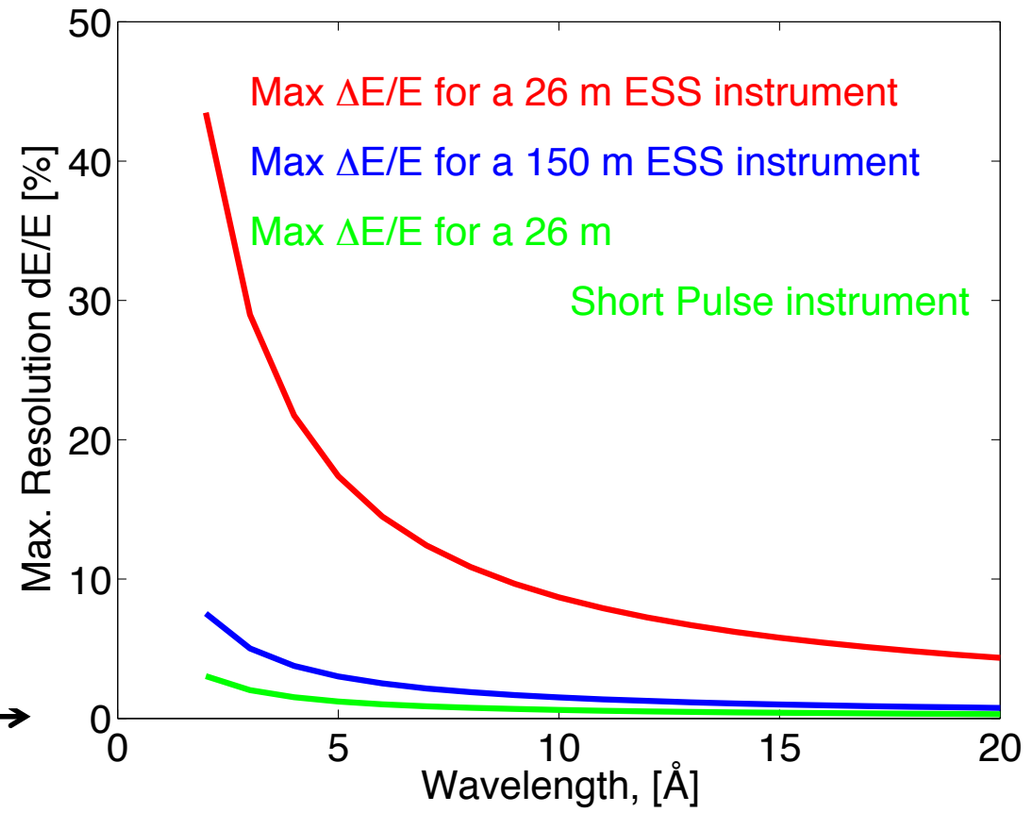

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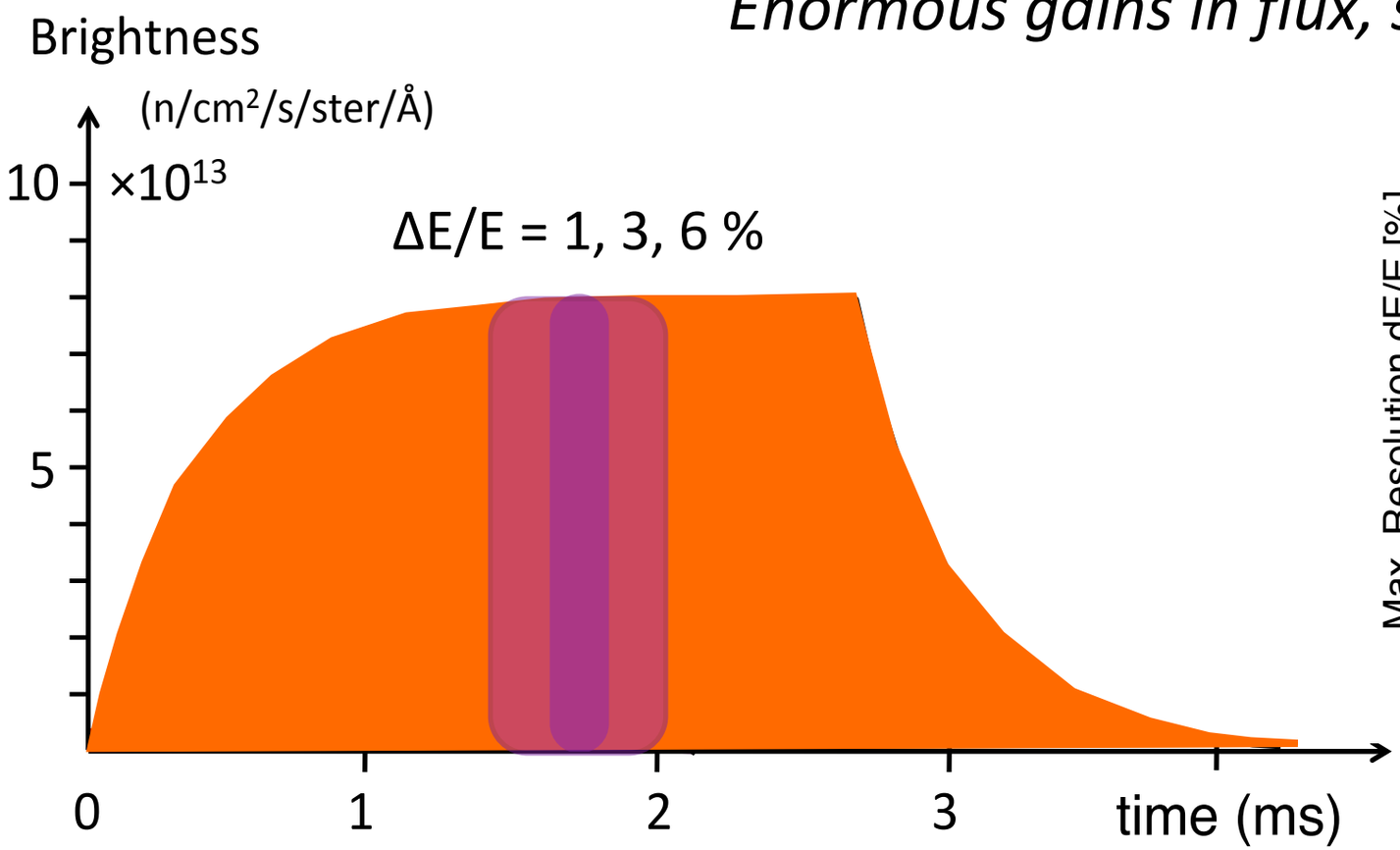

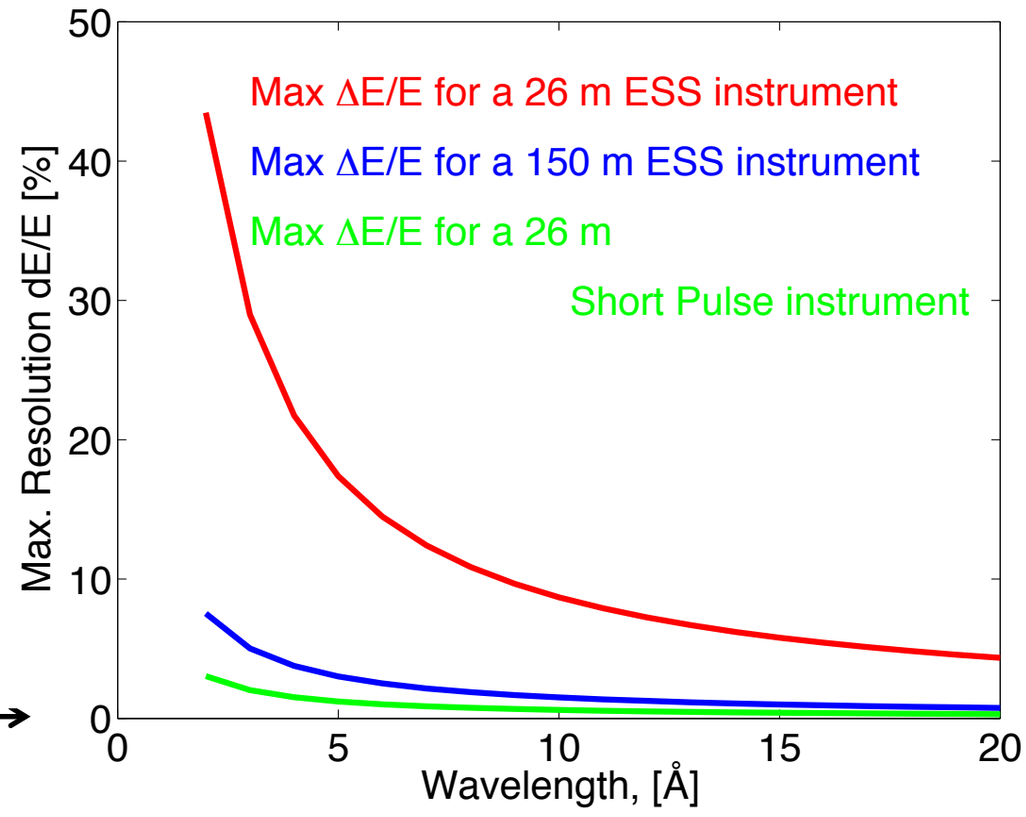

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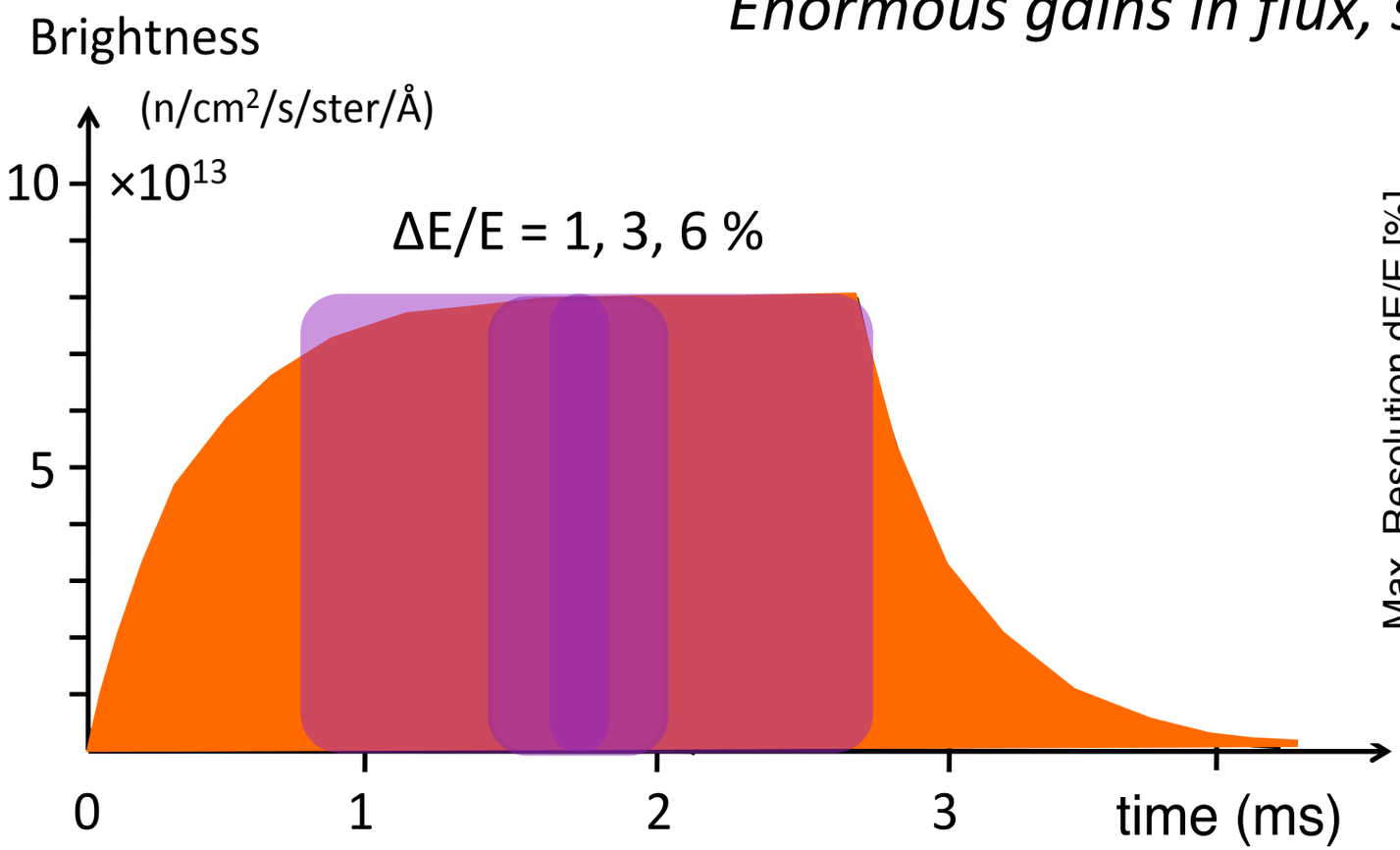

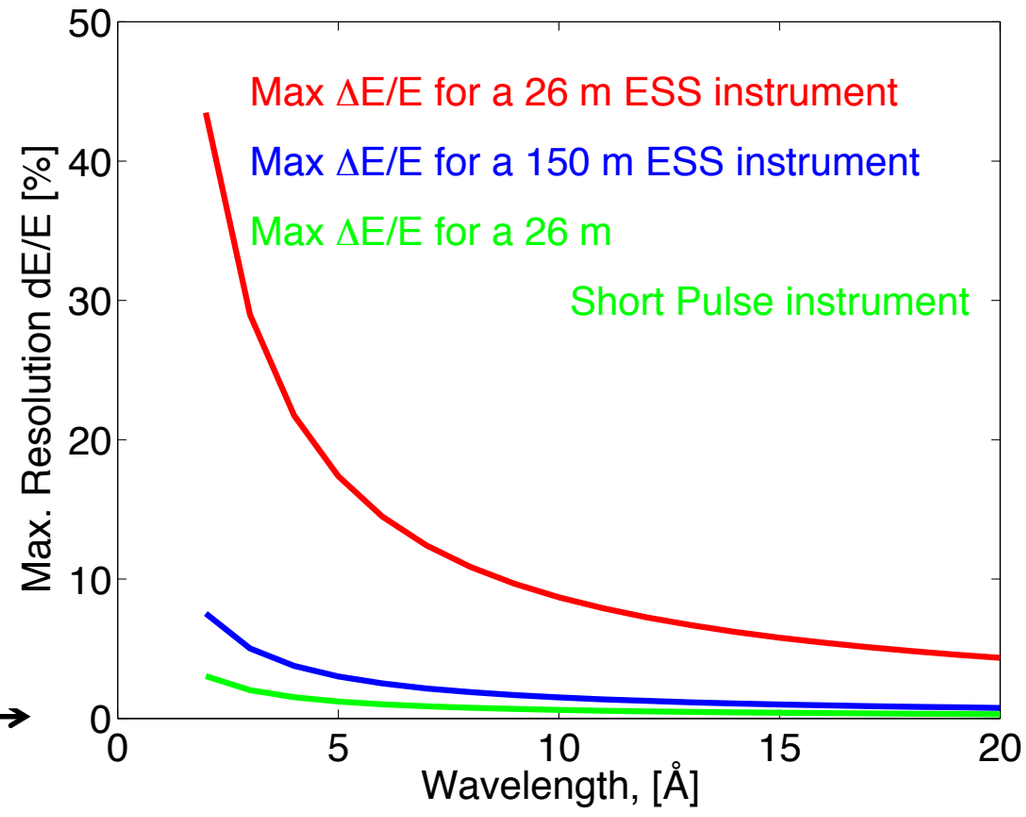

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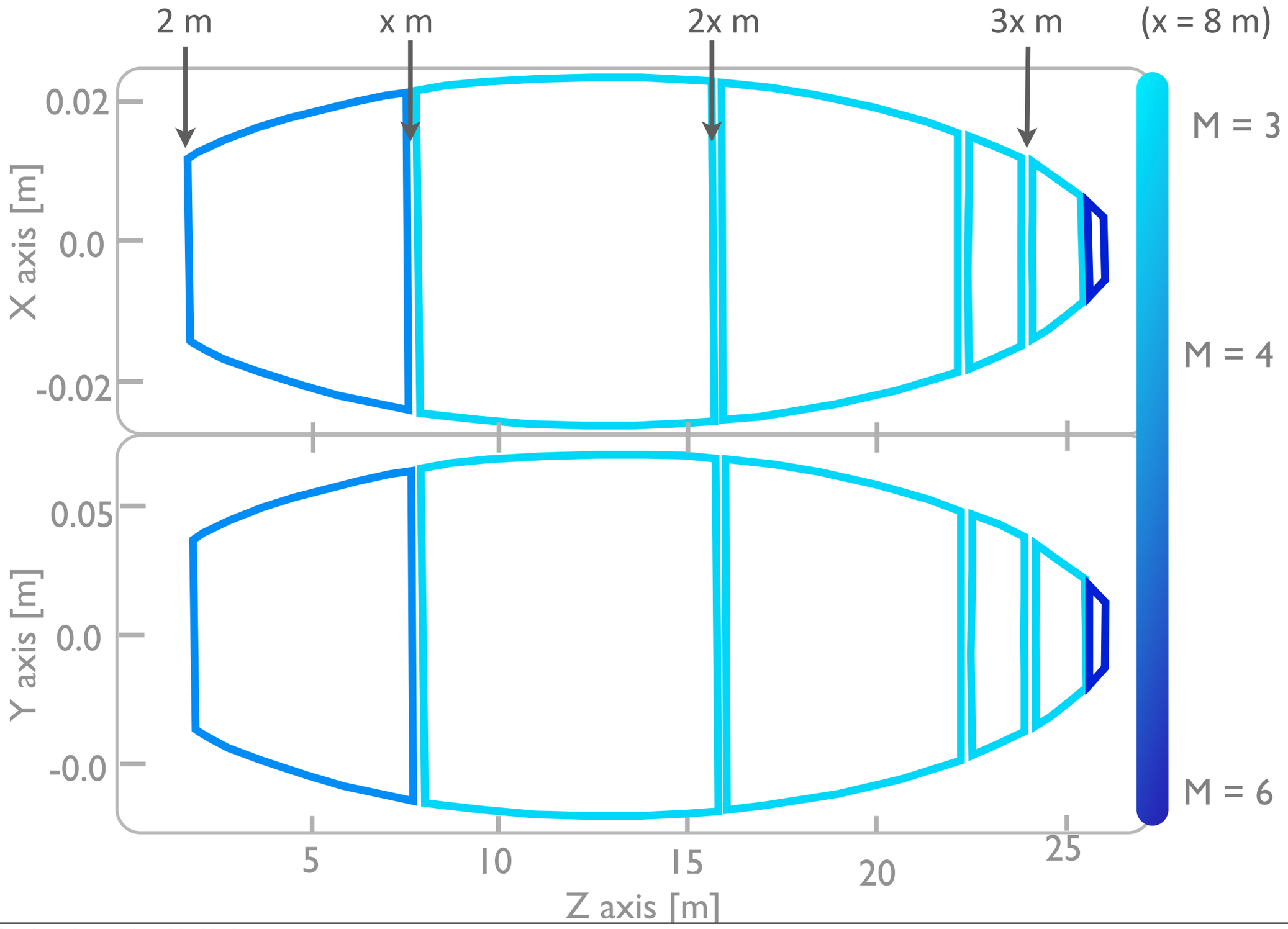
Guide concept

Straight ellipse

Ellipse: excellent focussing at the sample position

HEIGHT AXIS 7.1 CM ; WIDTH AXIS 2.5 CM



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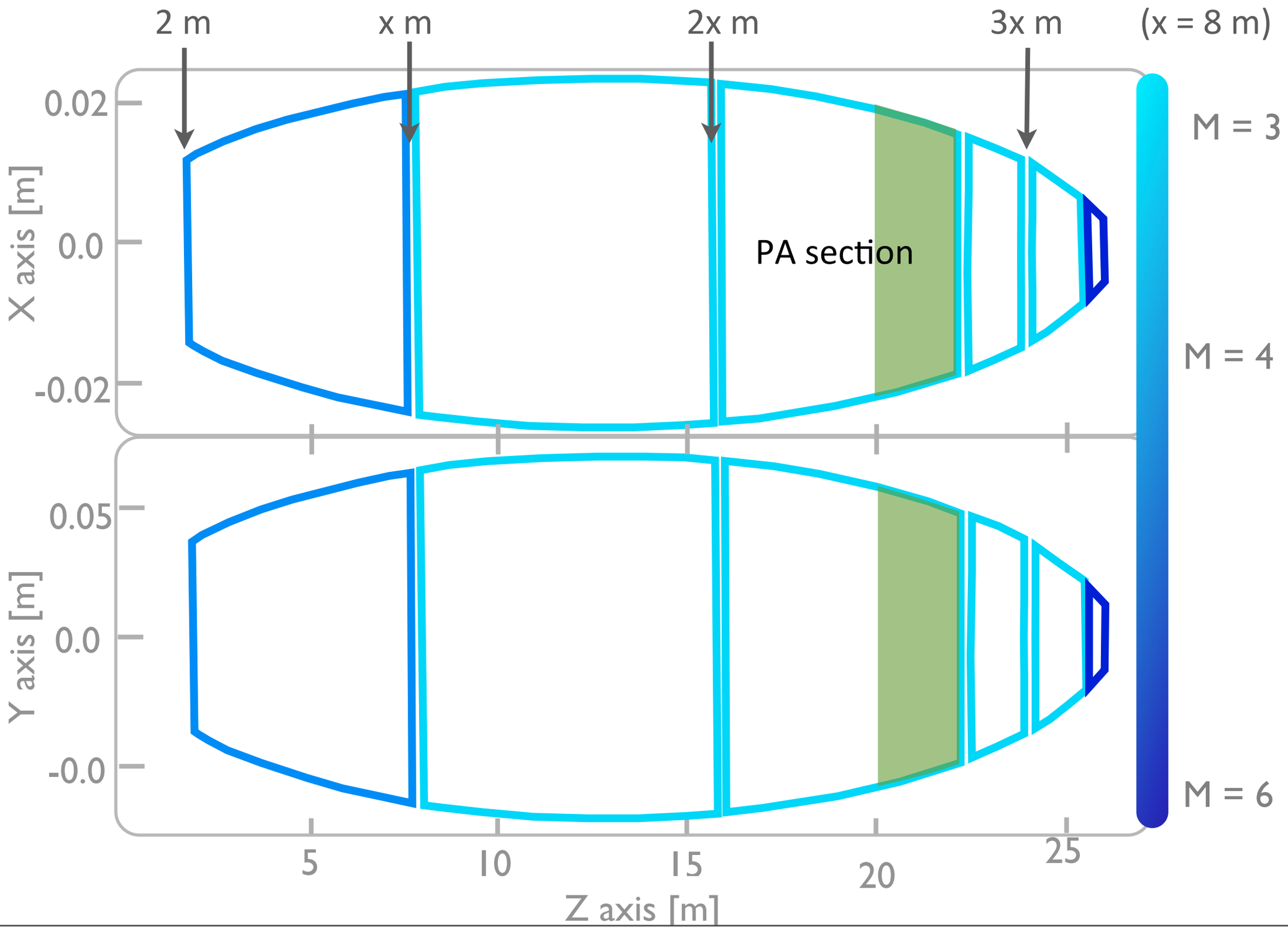

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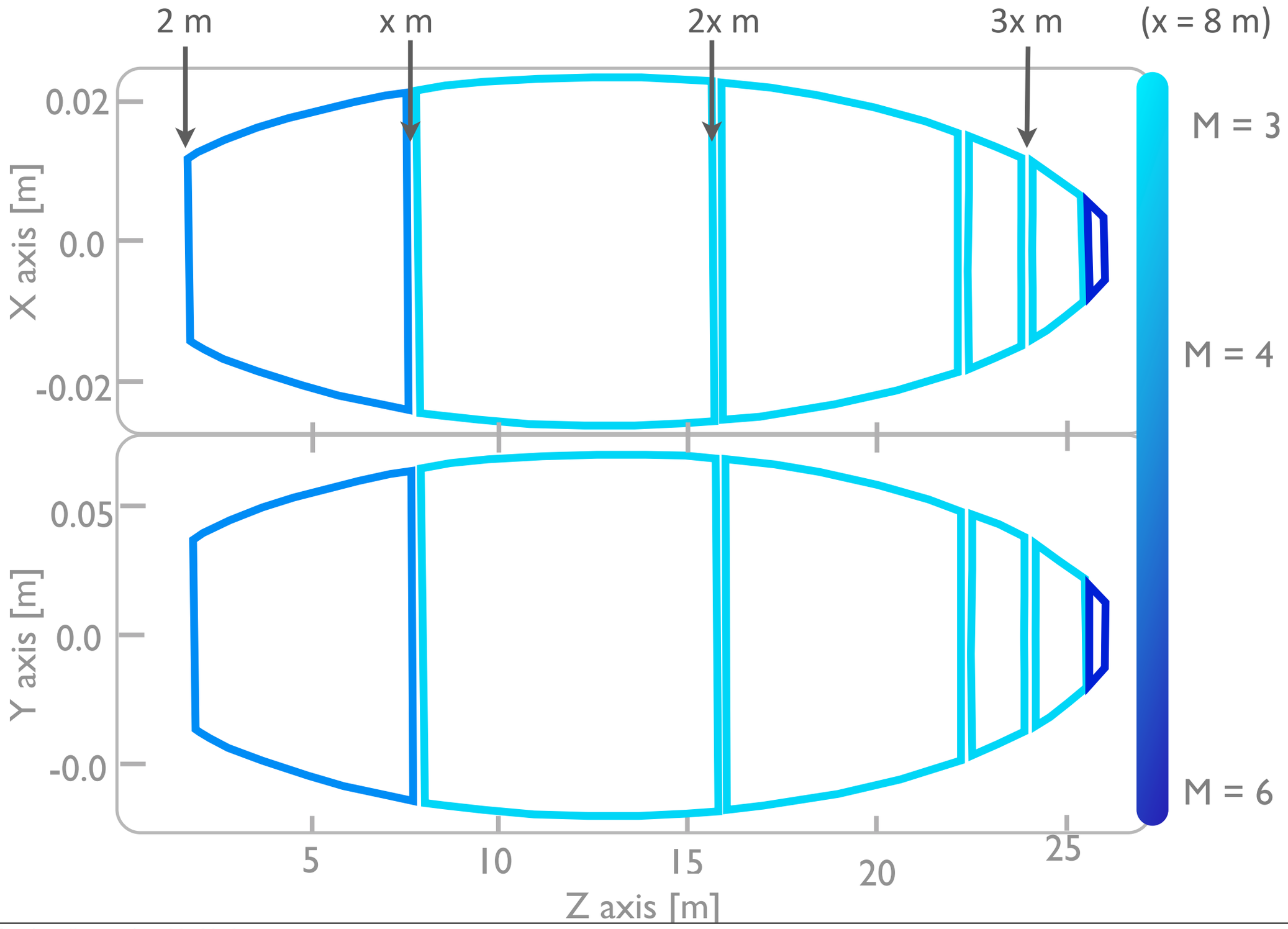

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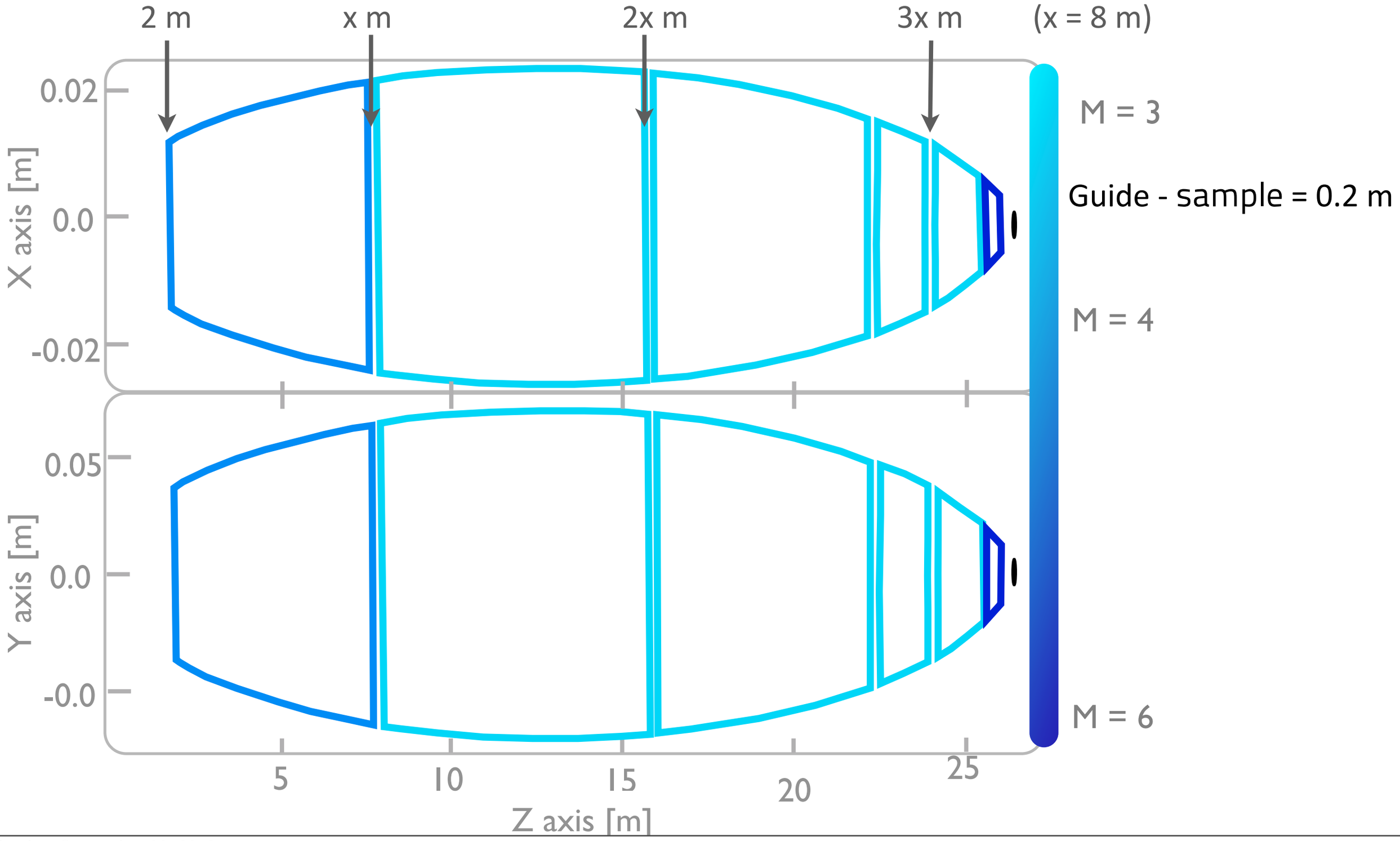

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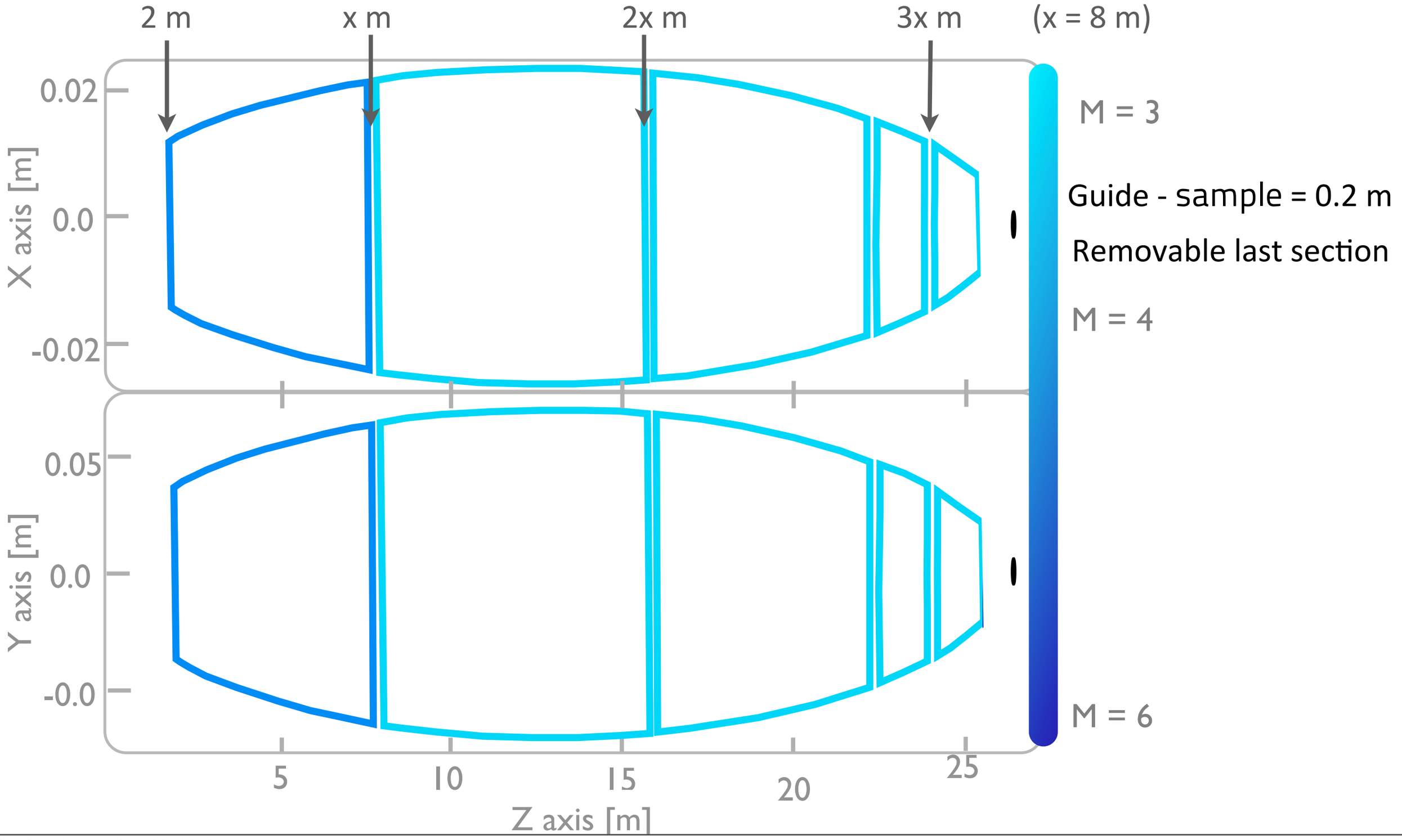

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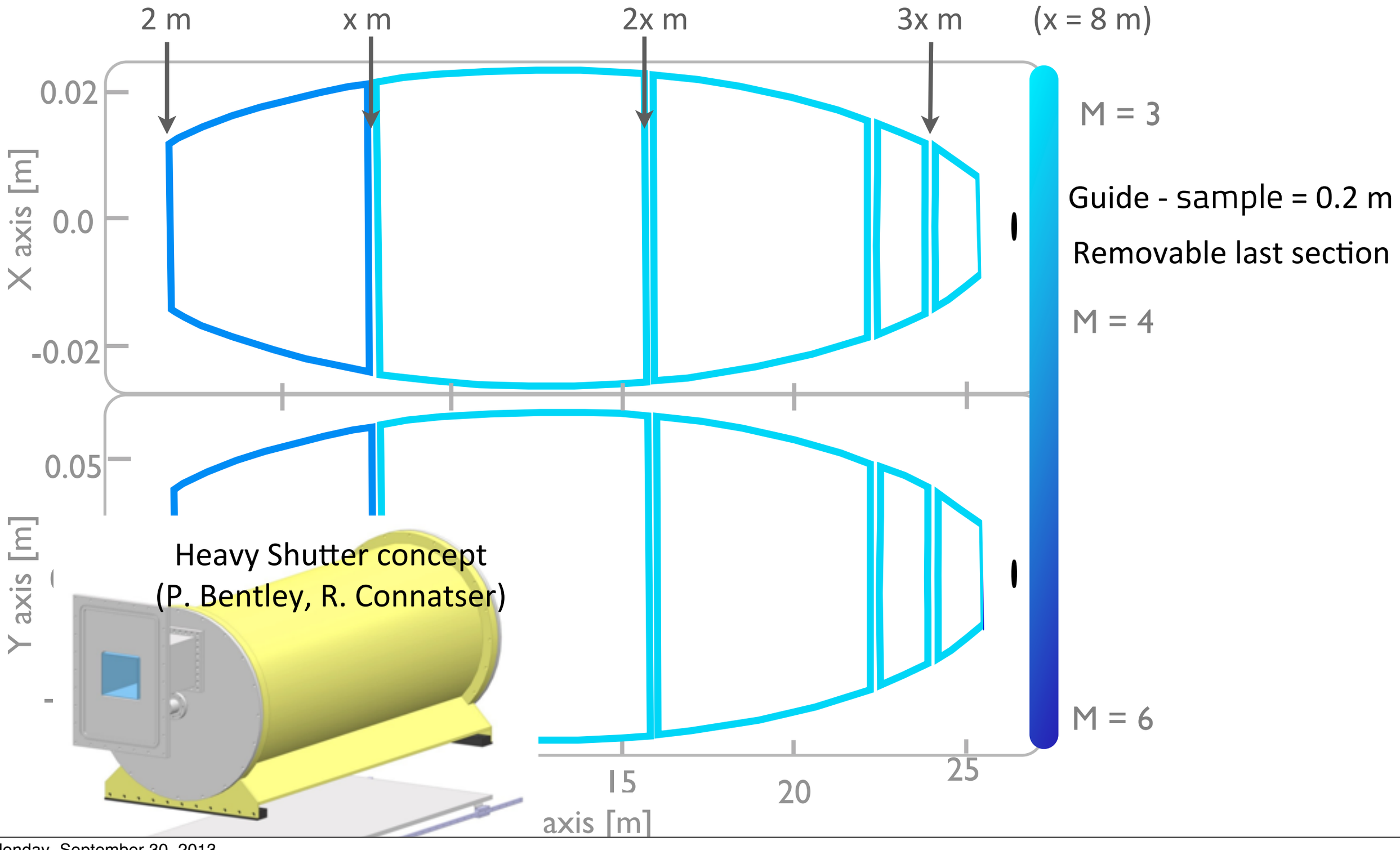
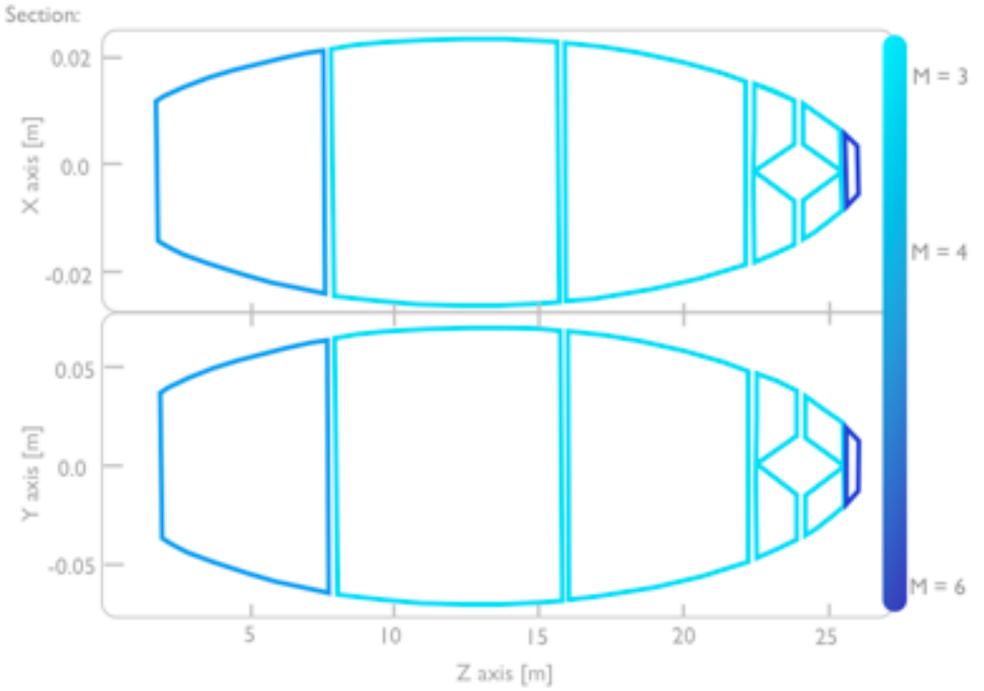
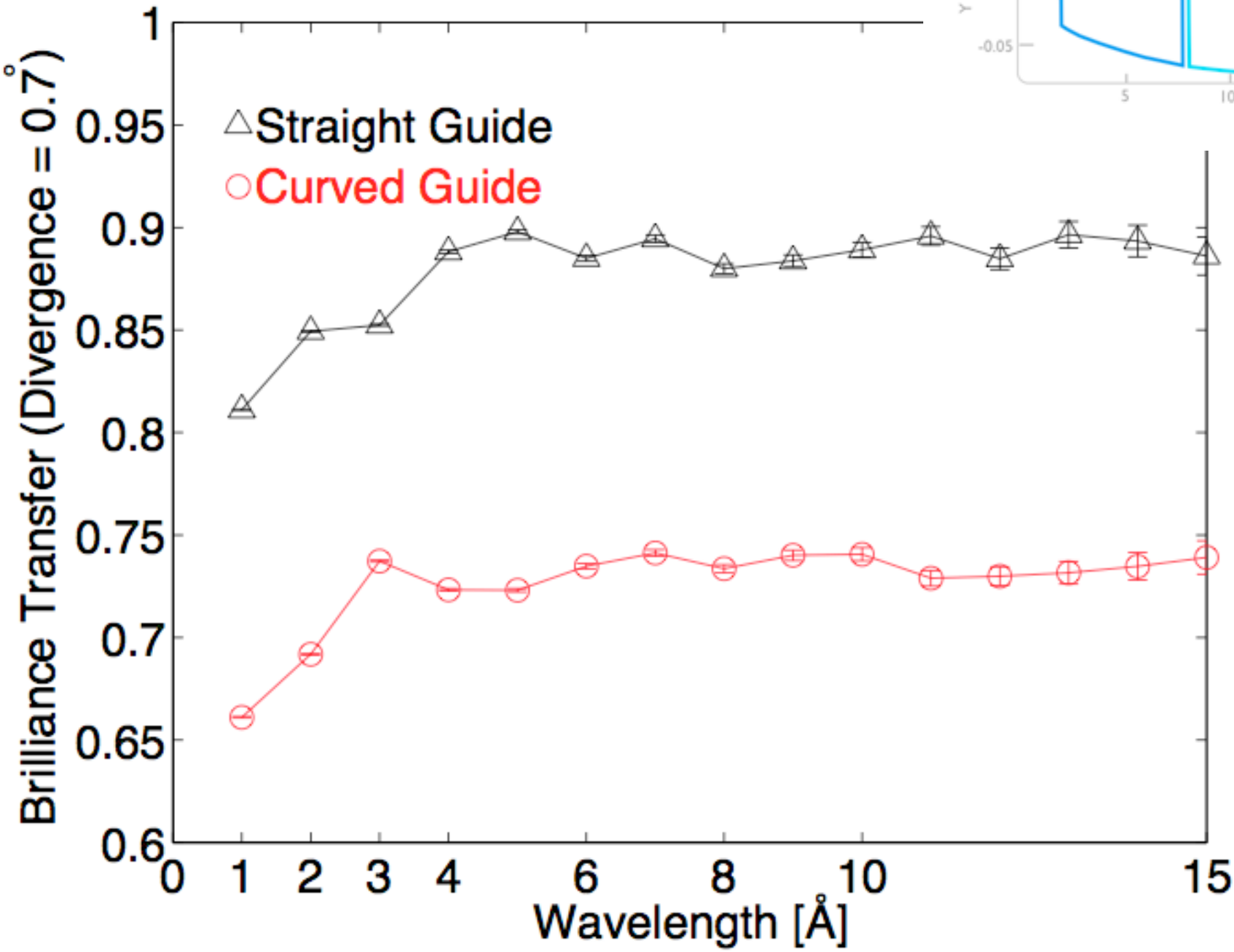


Heavy Shutter concept
(P. Bentley, R. Connatser)

EUROPEAN SPALLATION SOURCE

Guide concept



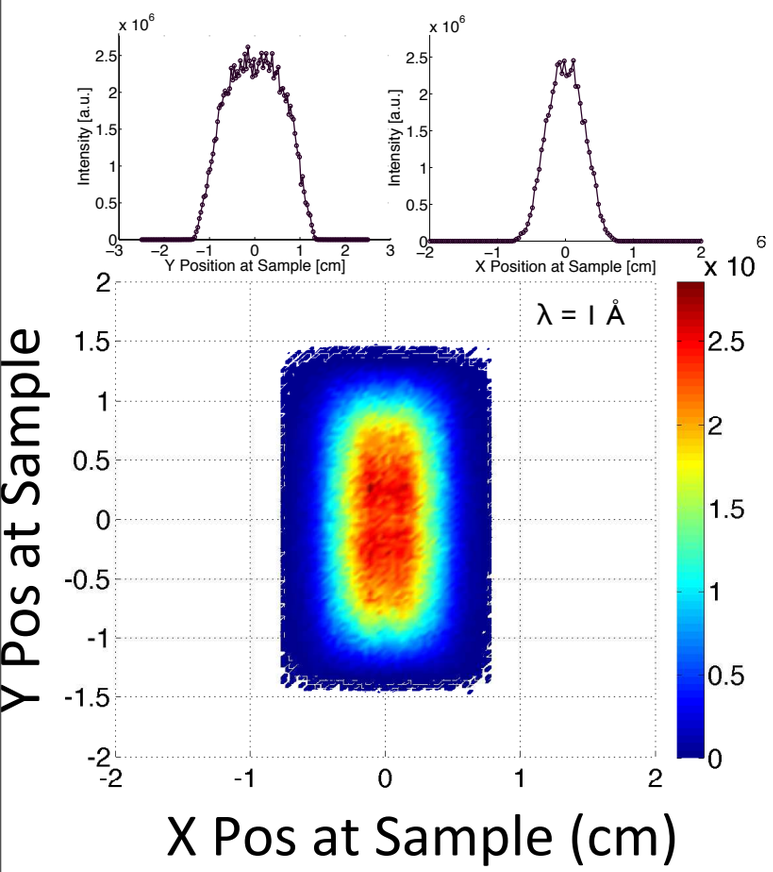


Beam Profiles (McStas)

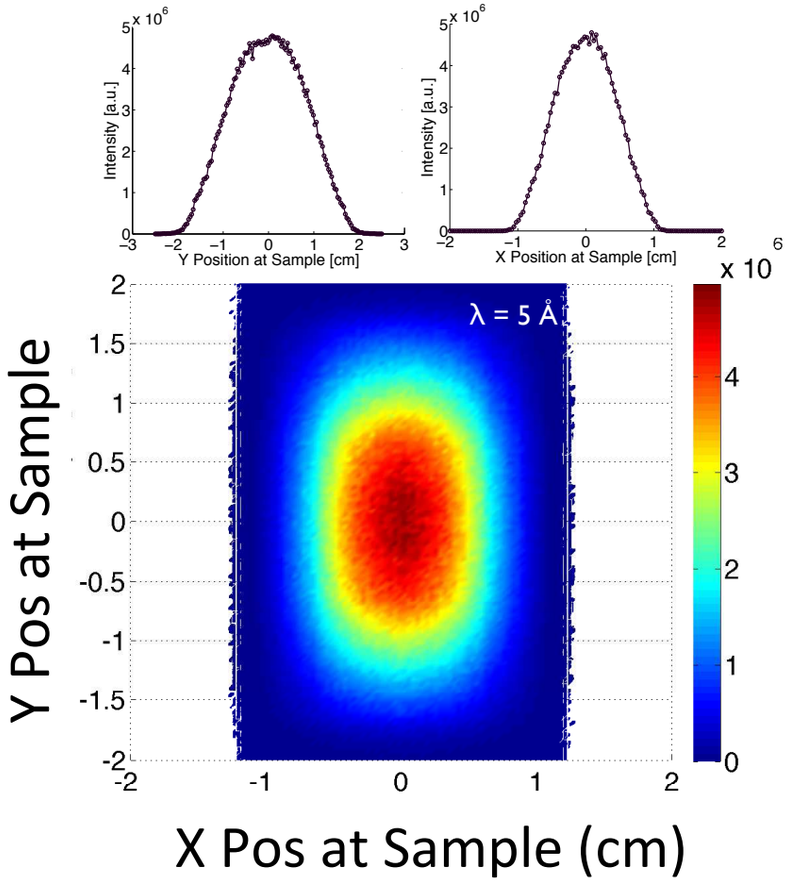
Requirements: Flat across sample area required (3 mm x 1 cm).
Clean divergence profile.

Flux

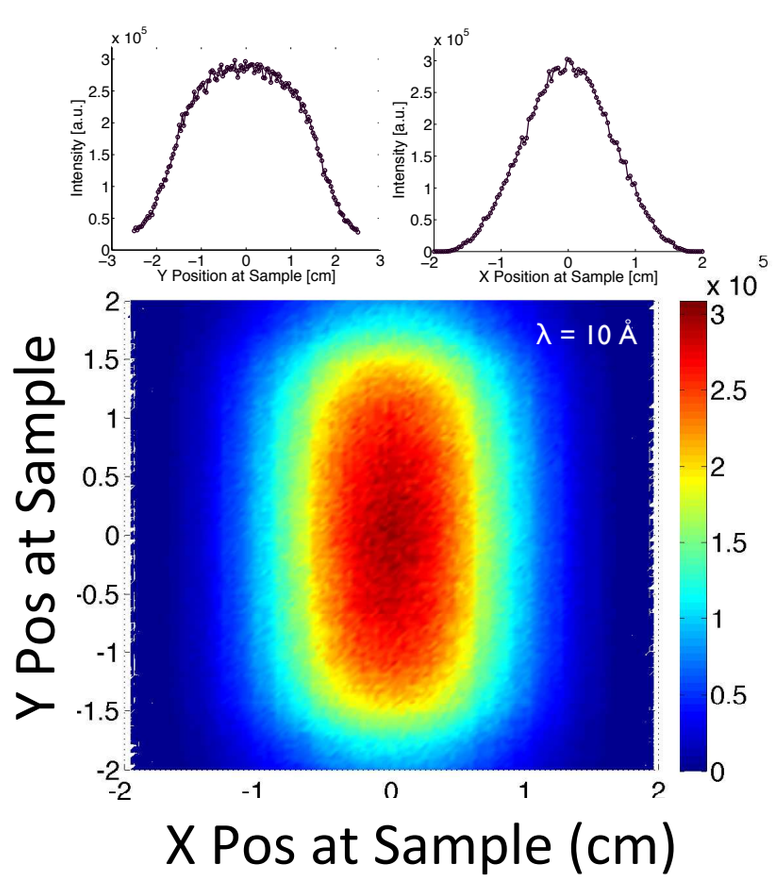
1 Å



5 Å



10 Å



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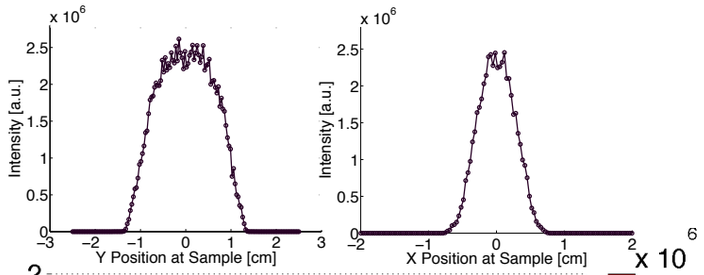
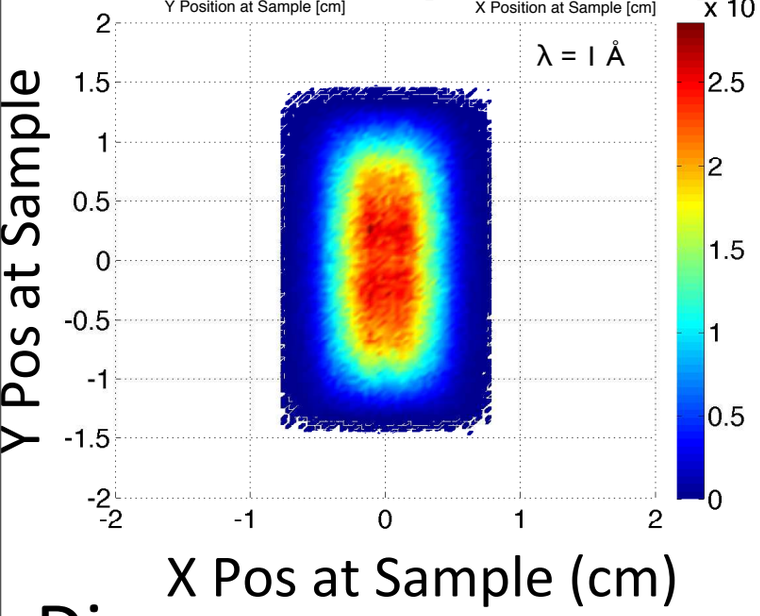
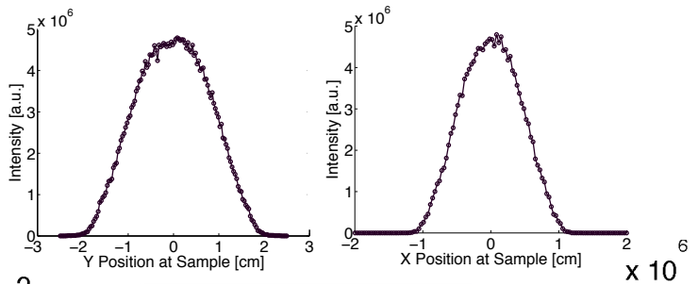
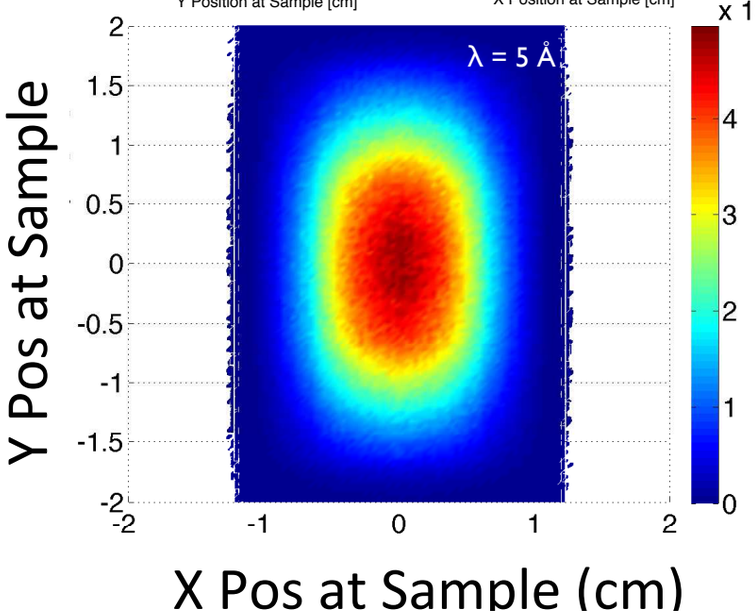


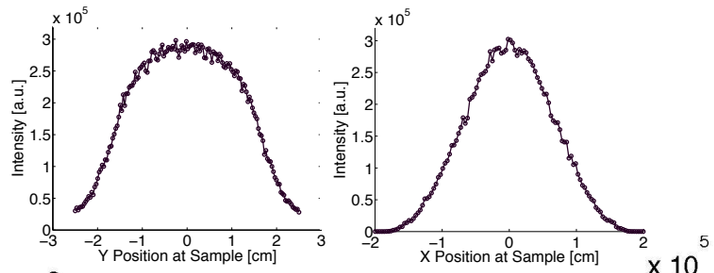


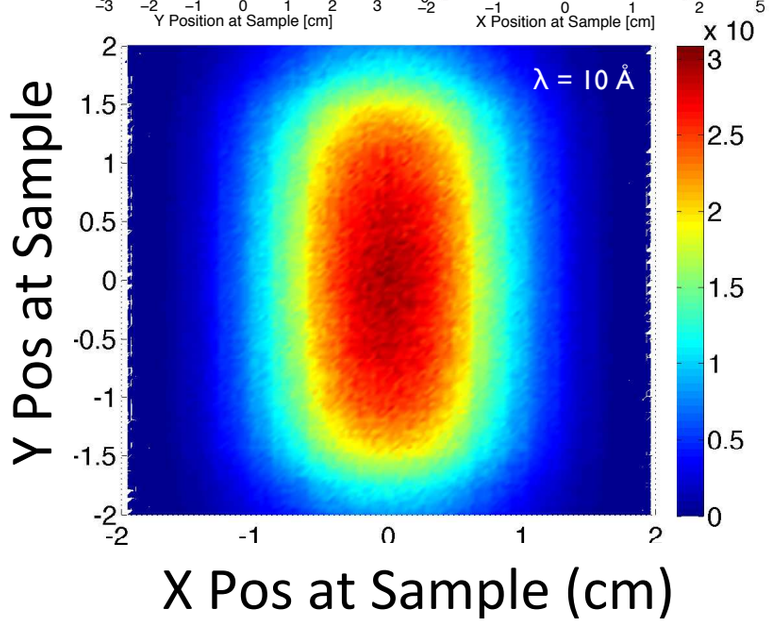
5 Å



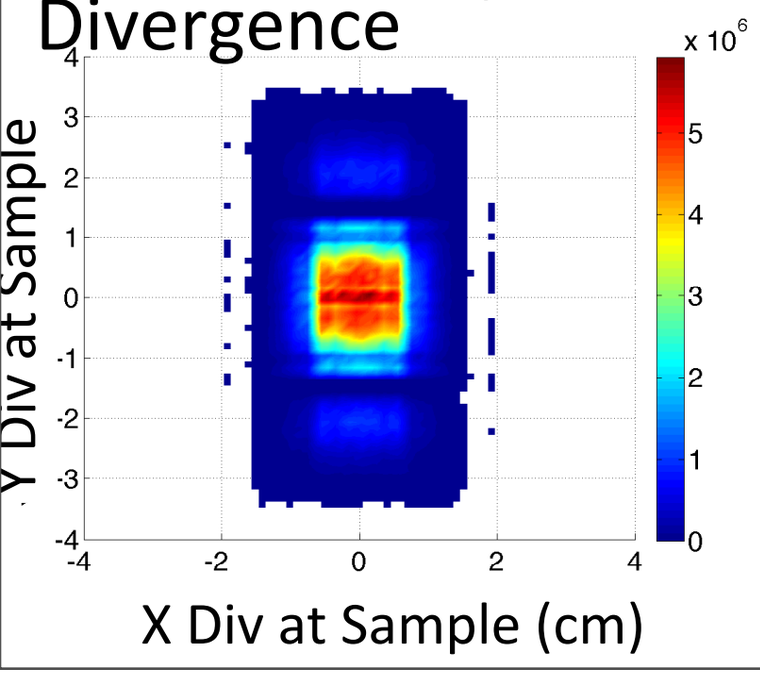


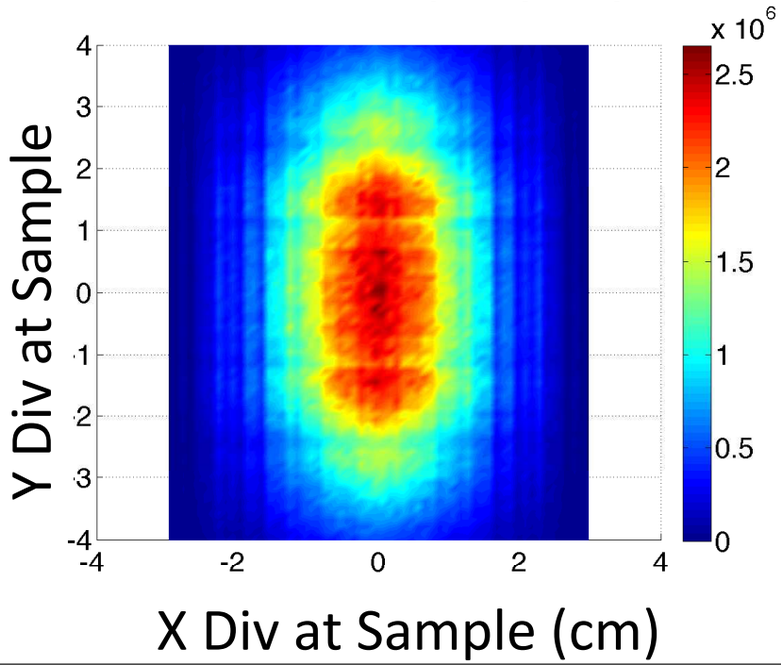
10 Å

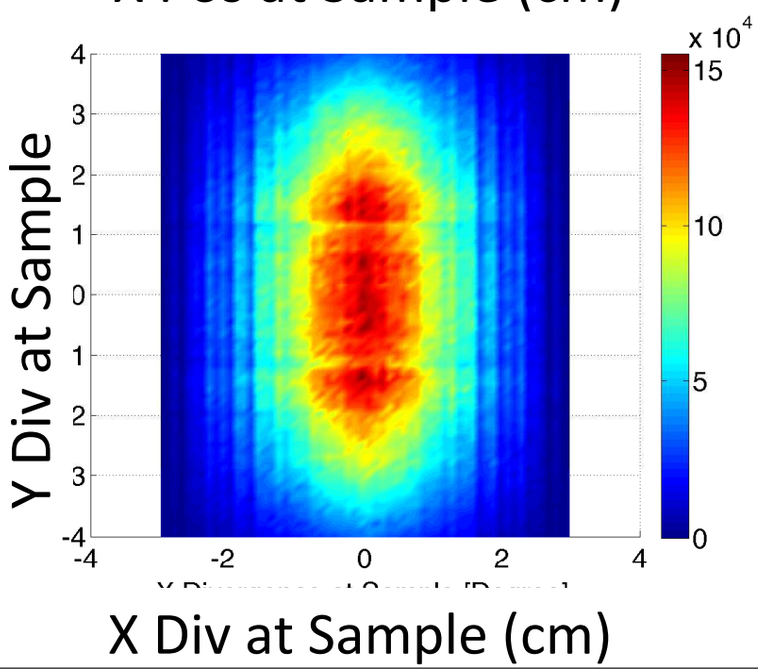




Divergence







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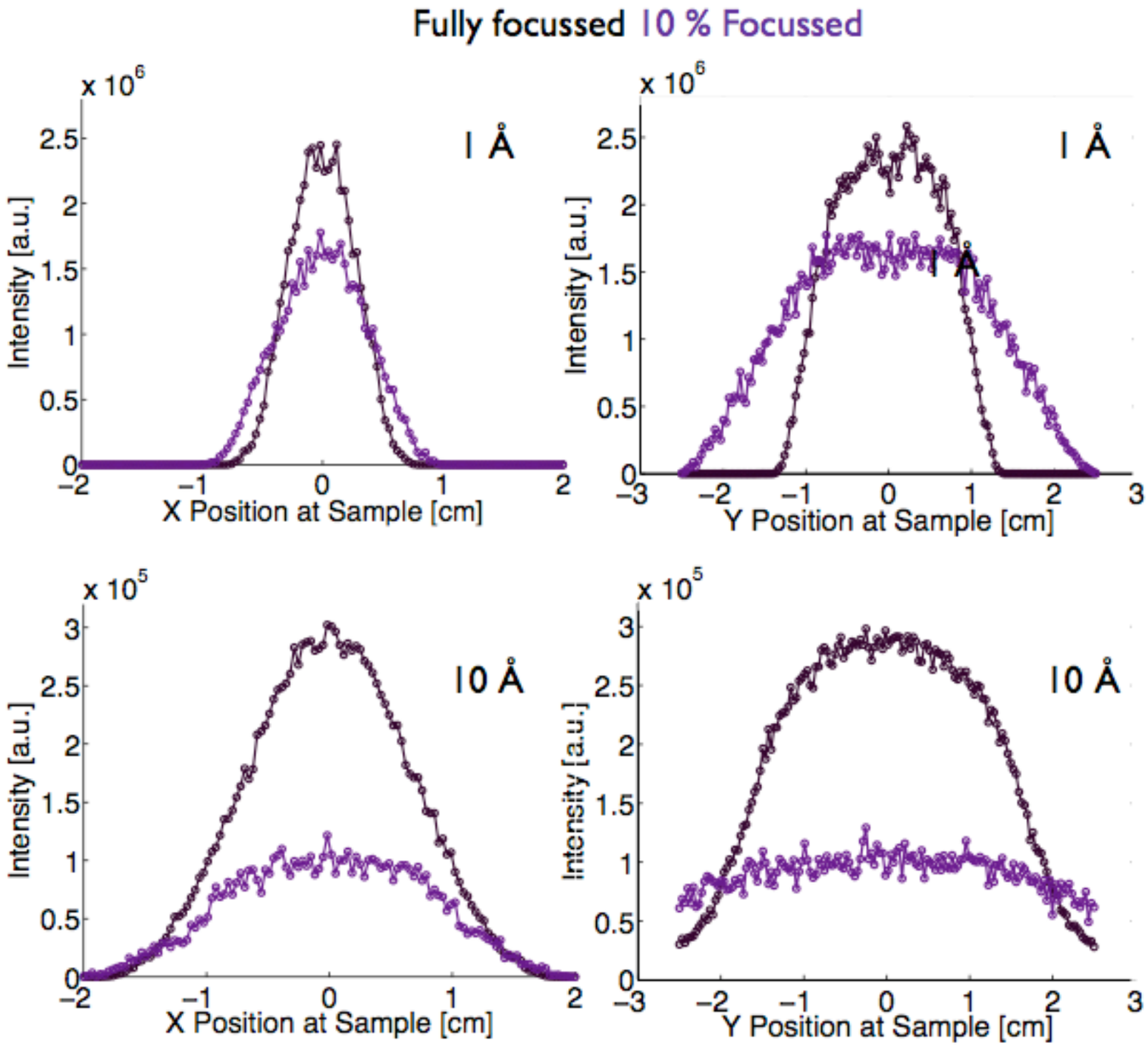
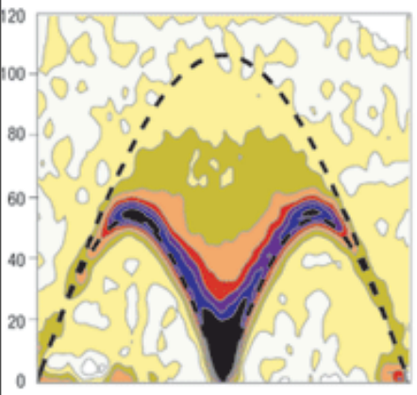
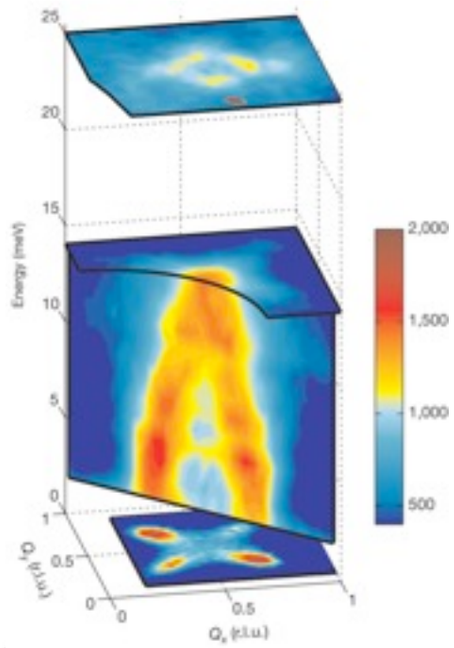
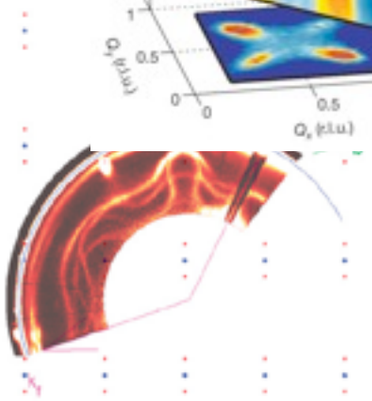


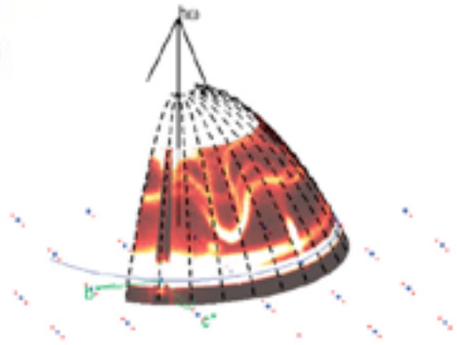
3 mm x 1 cm ⇒ 3 mm x 2 cm - loose a factor of 3 in flux.

EUROPEAN SPALLATION SOURCE

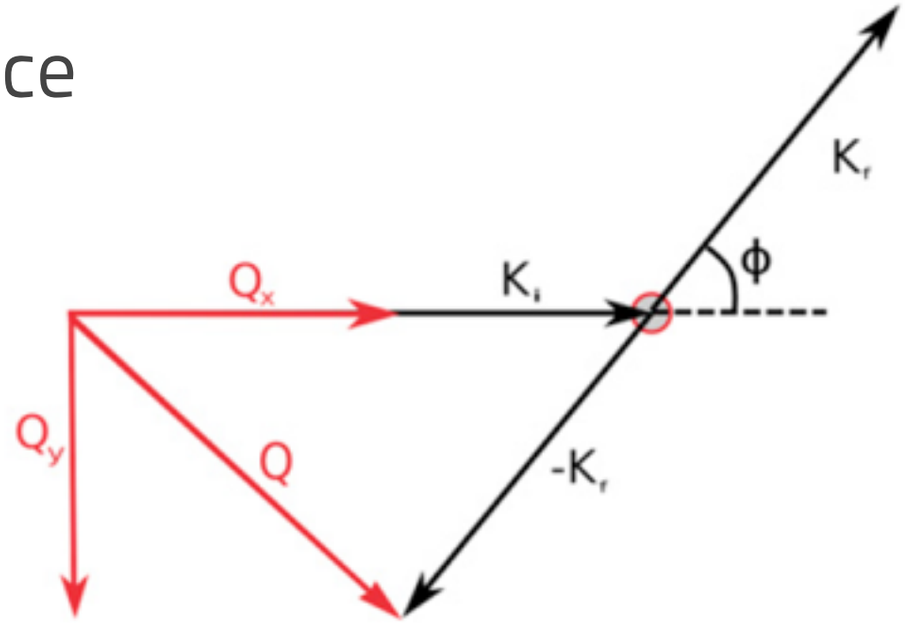




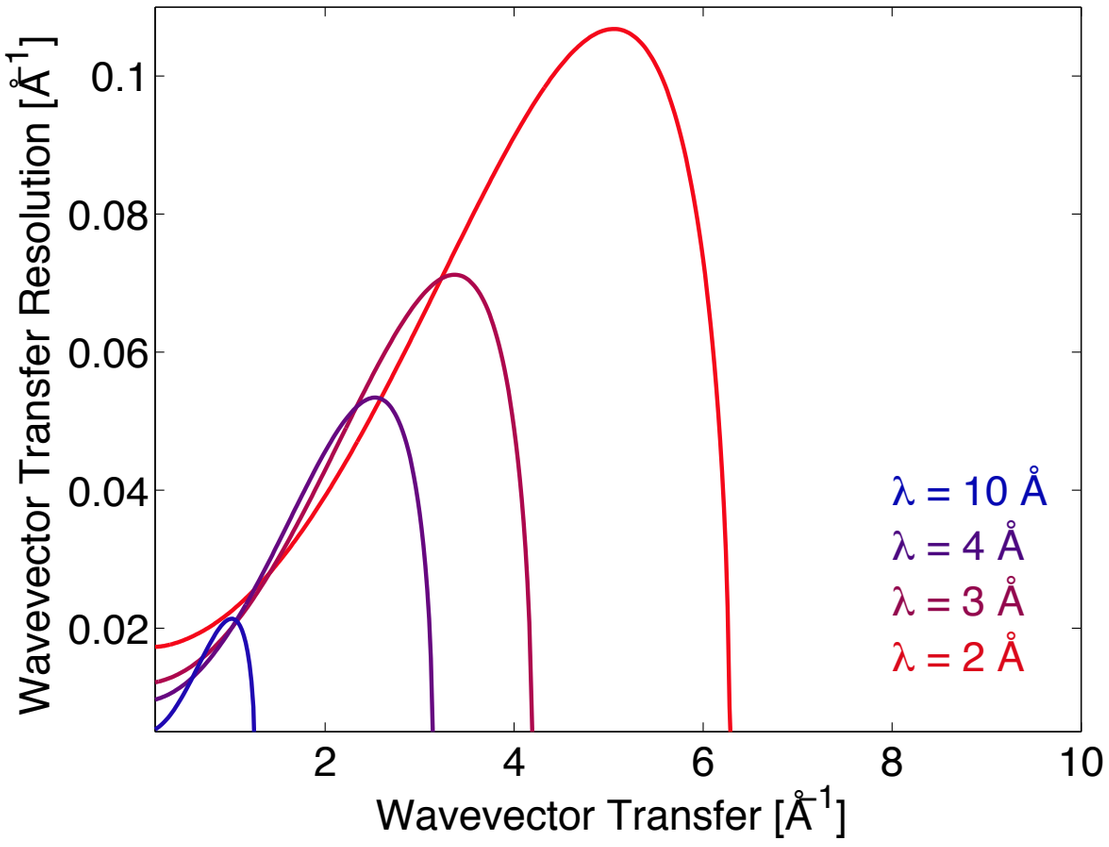




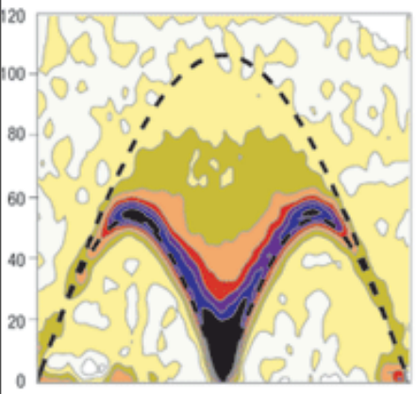
Q-dependence

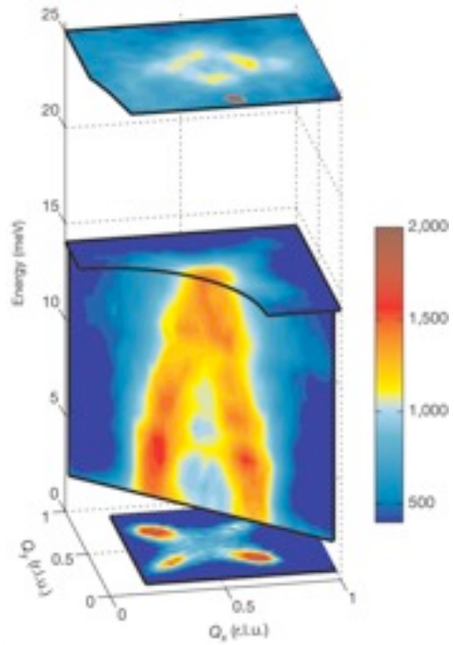


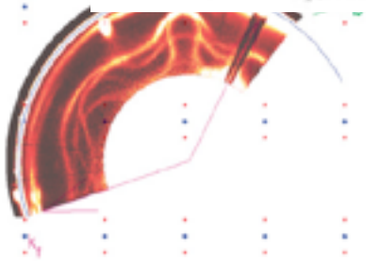
VOR

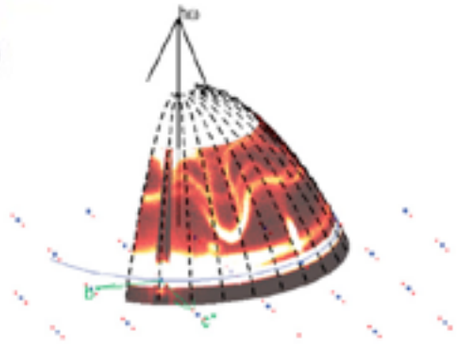


EUROPEAN SPALLATION SOURCE









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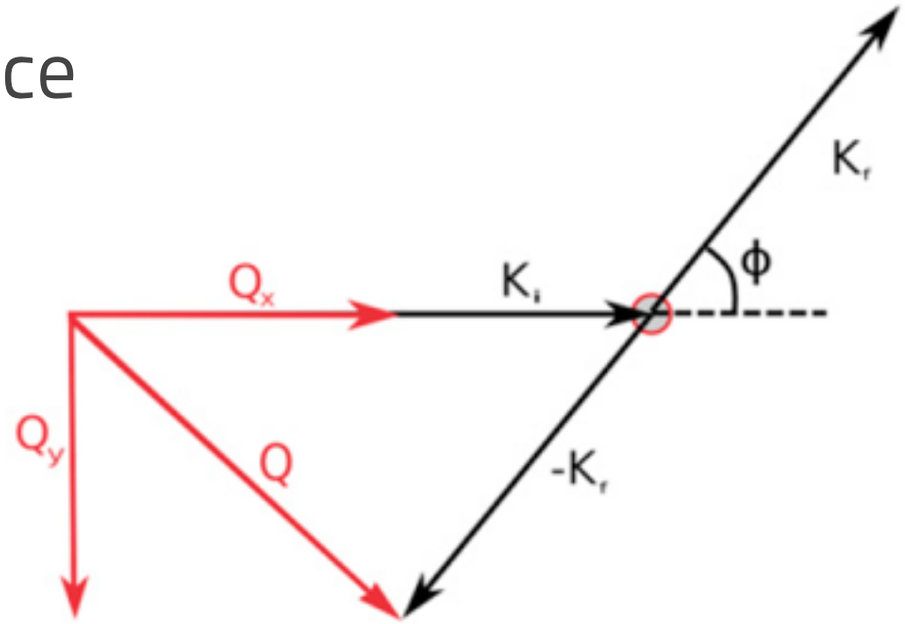
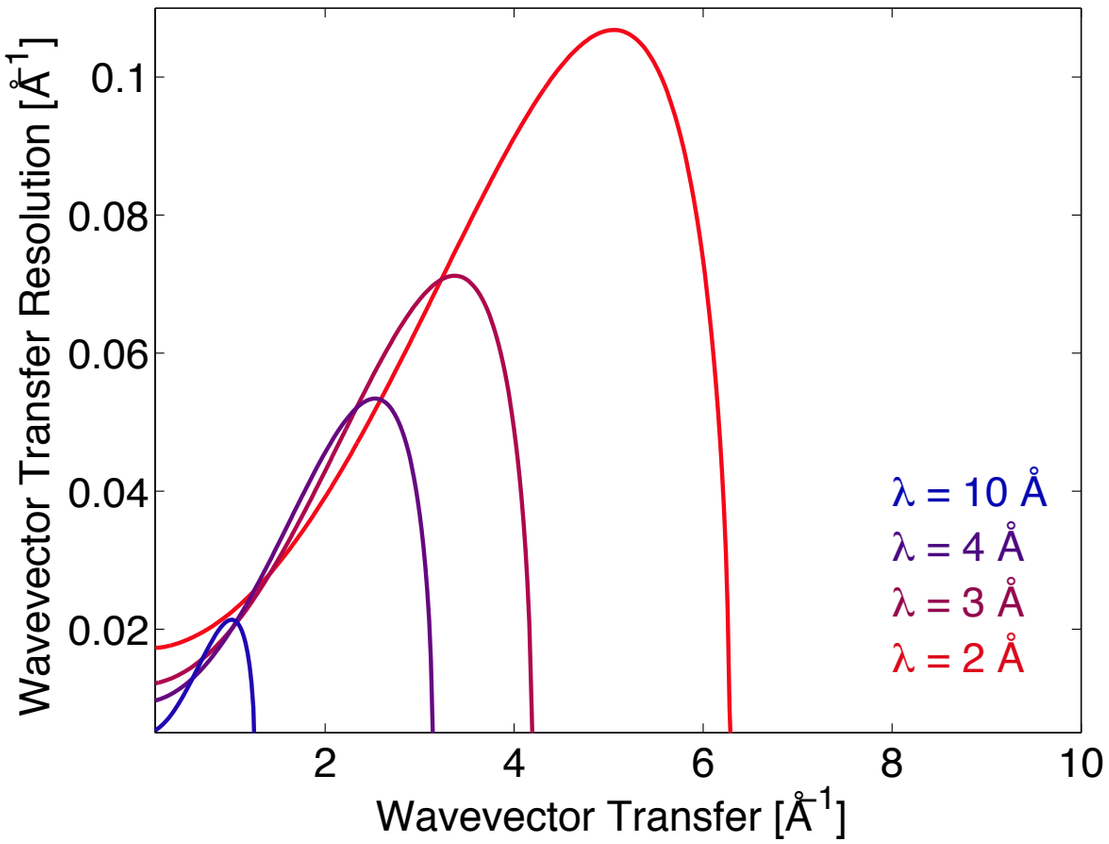
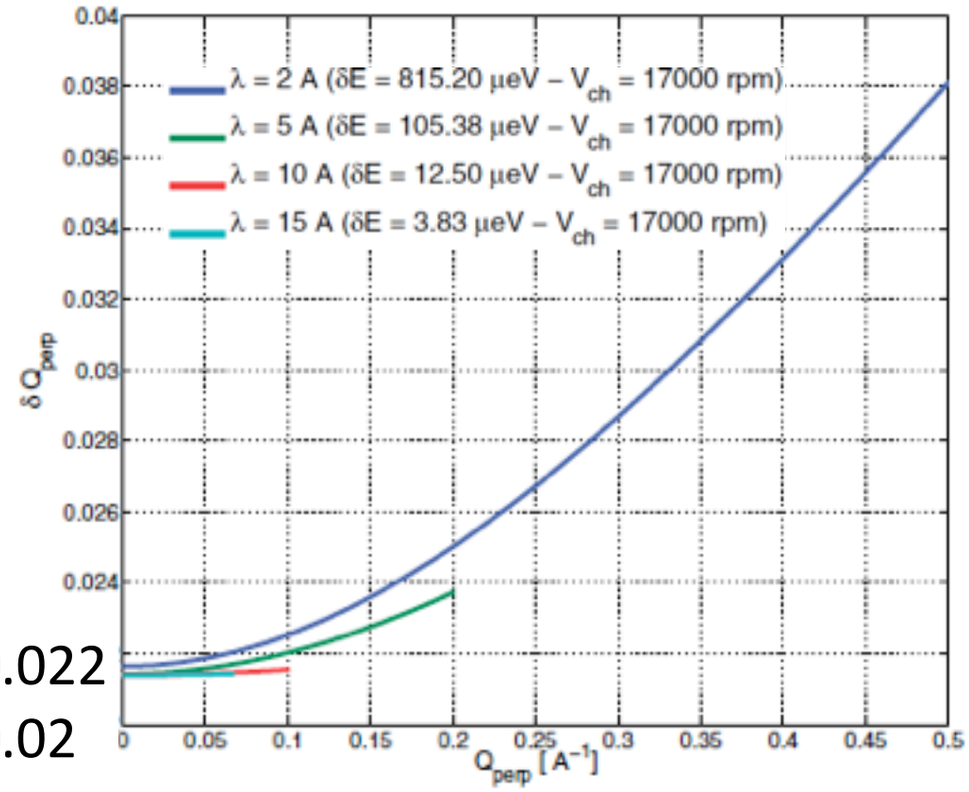


VOR

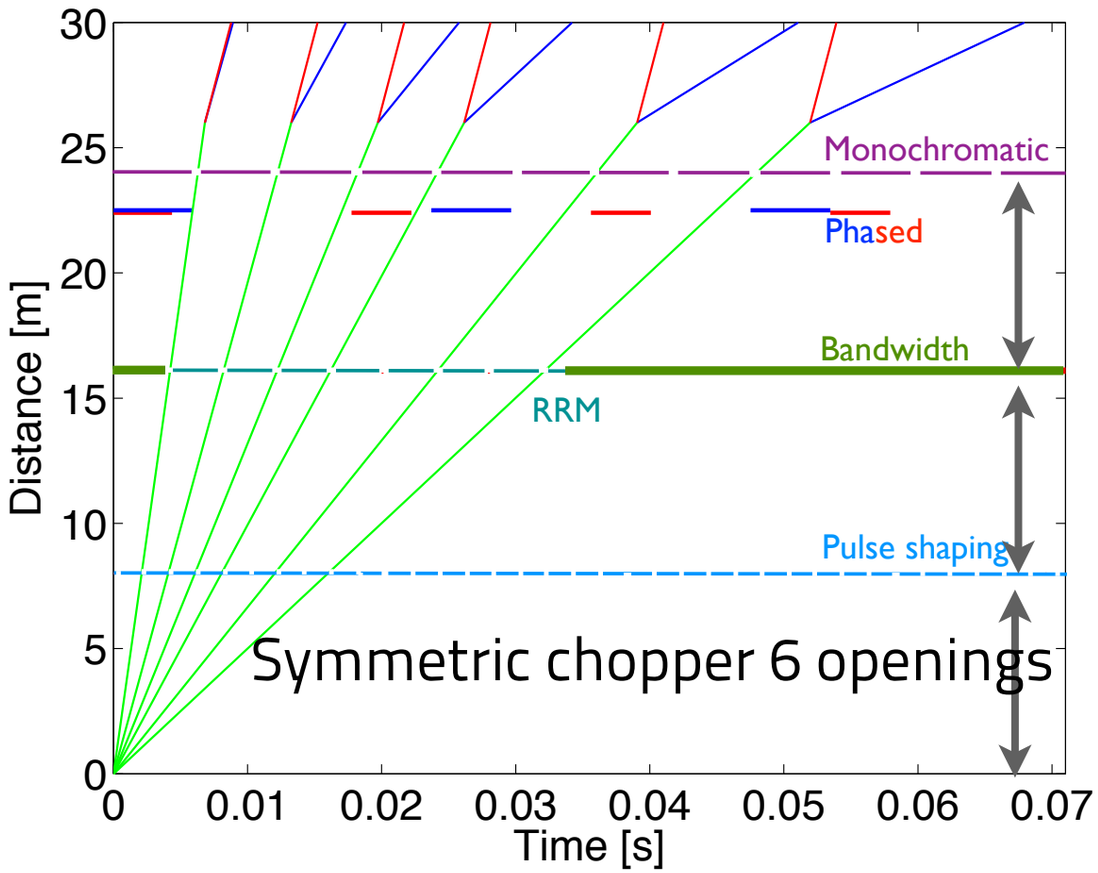


IN5



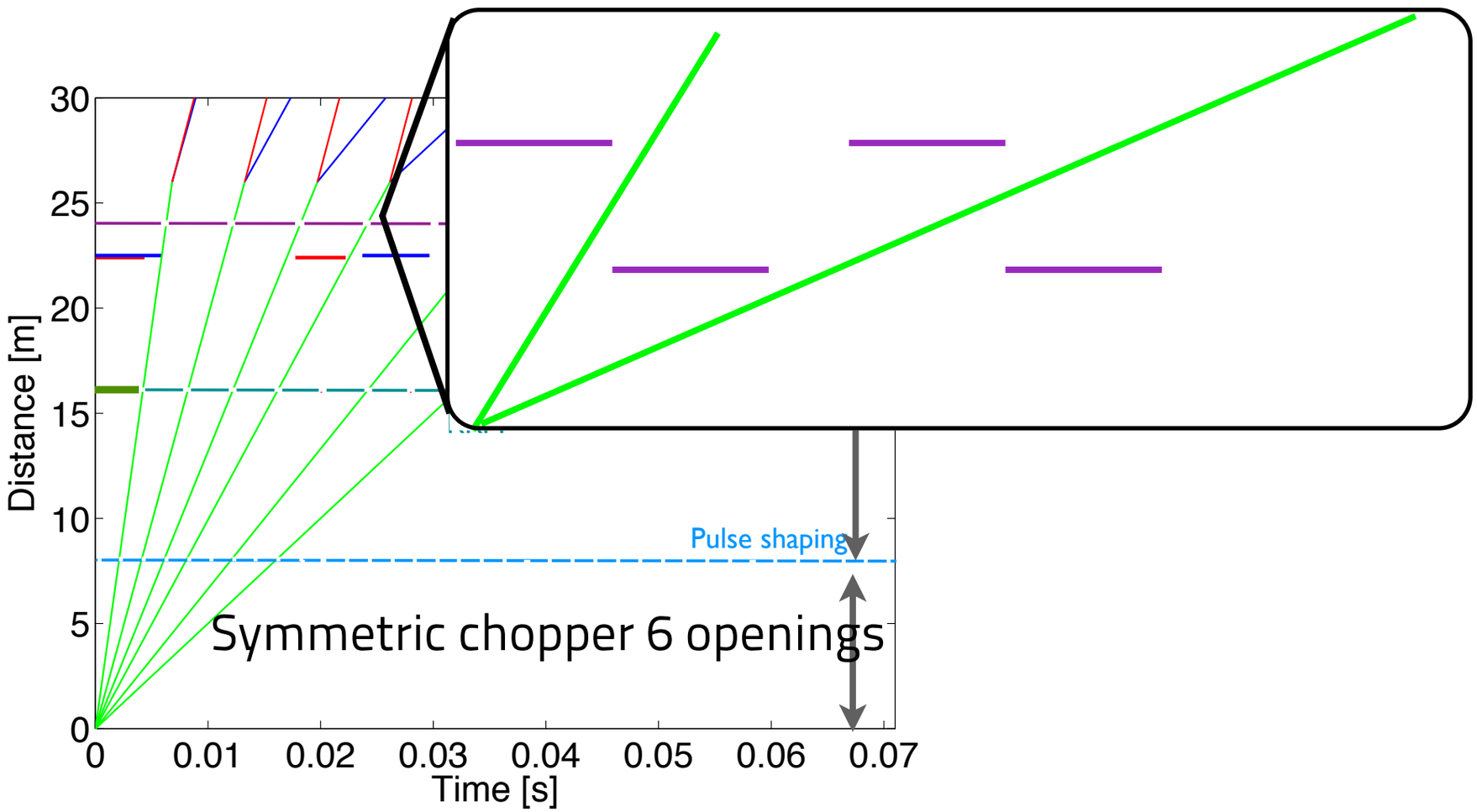
General Chopper set-up
RRM in mind (X:2X:3X)
Chopper dimensions and speeds are all currently available

Symmetric chopper 4 openings



EUROPEAN SPALLATION SOURCE

General Chopper set-up
RRM in mind (X:2X:3X)
Chopper dimensions and speeds are all currently available



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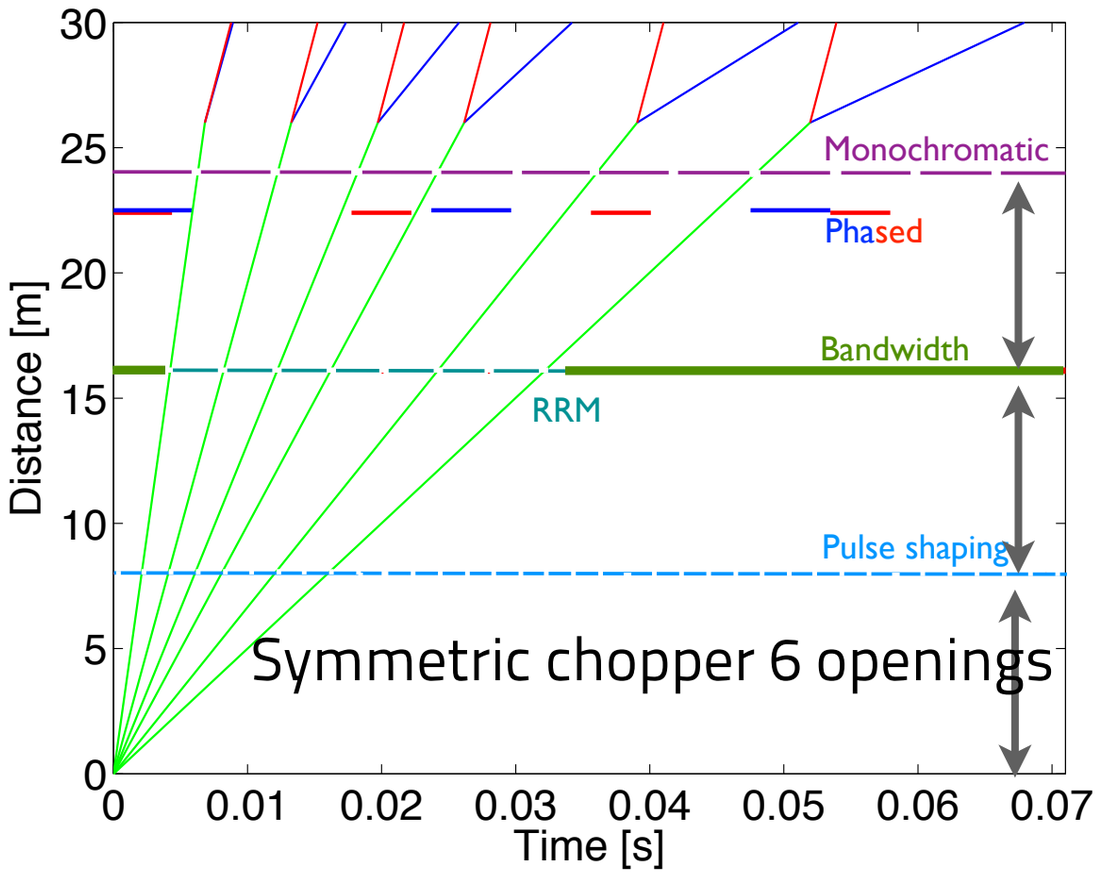

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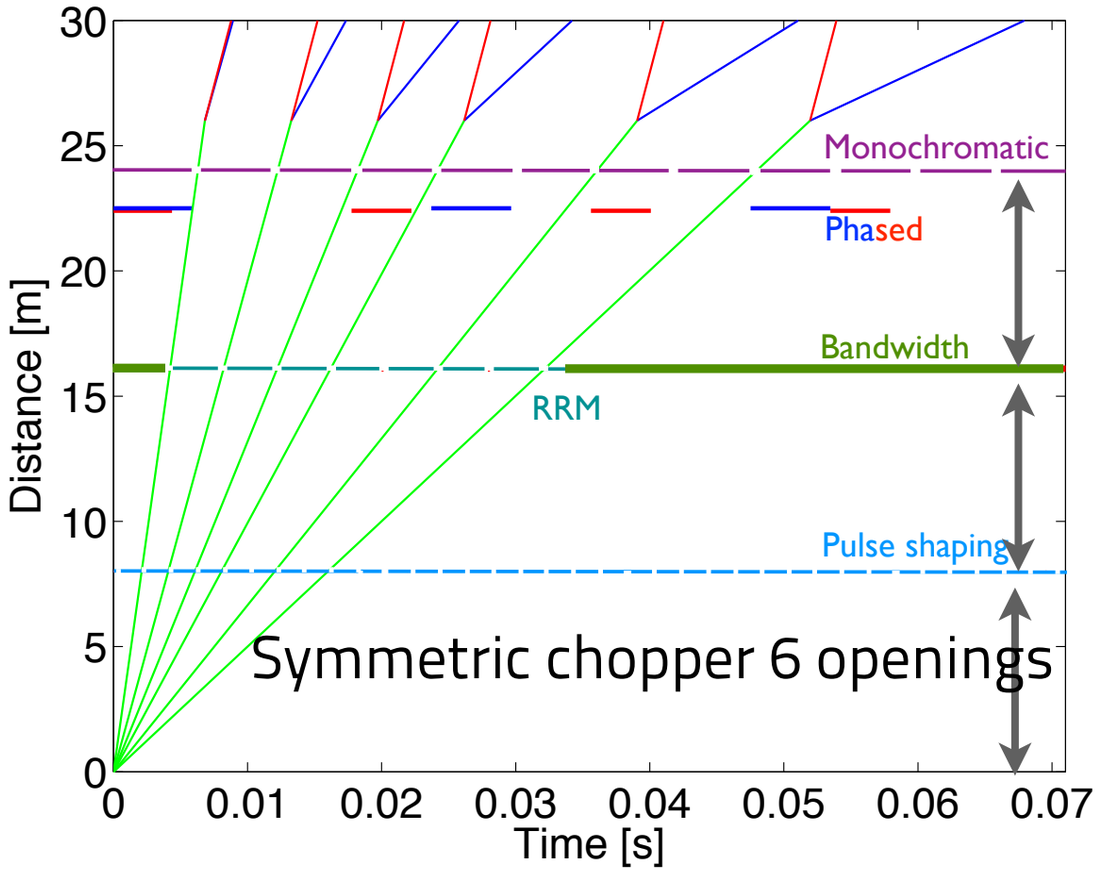
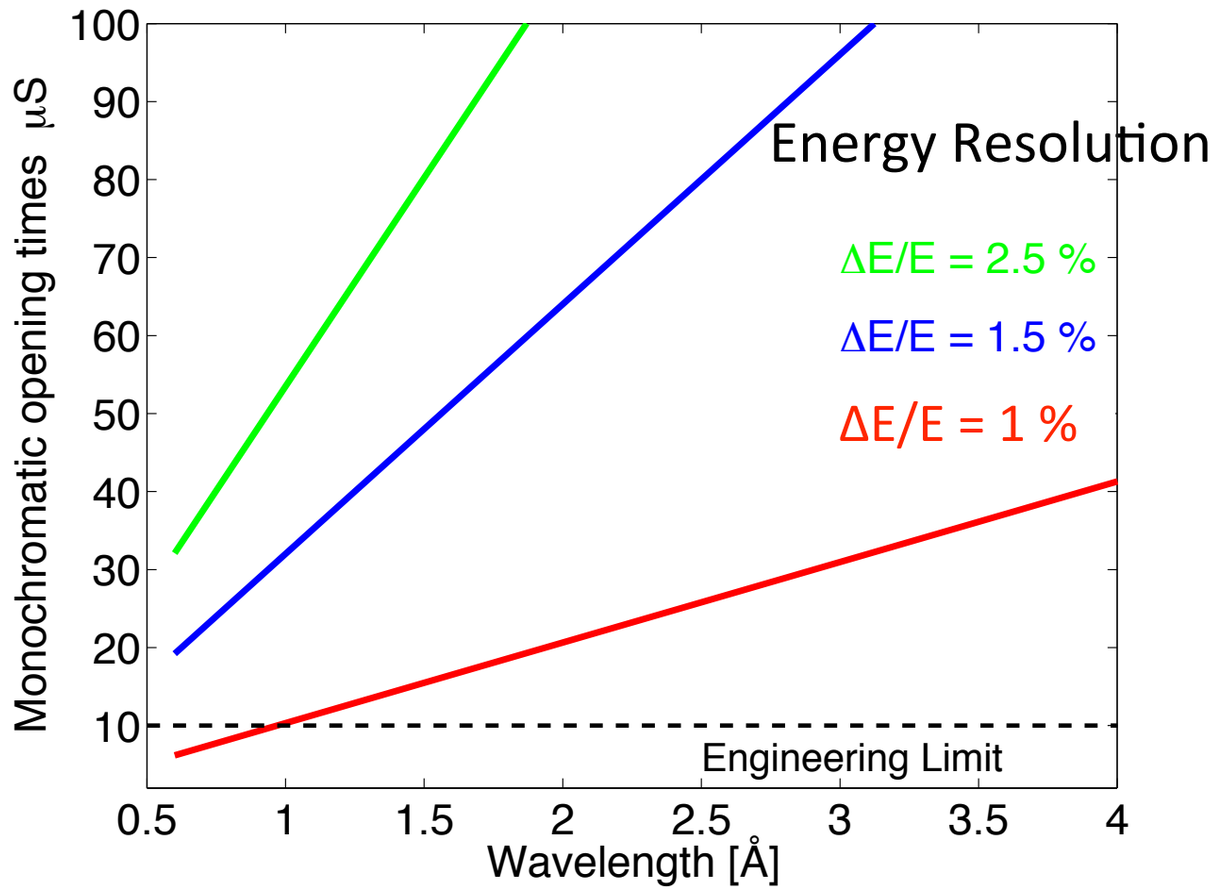
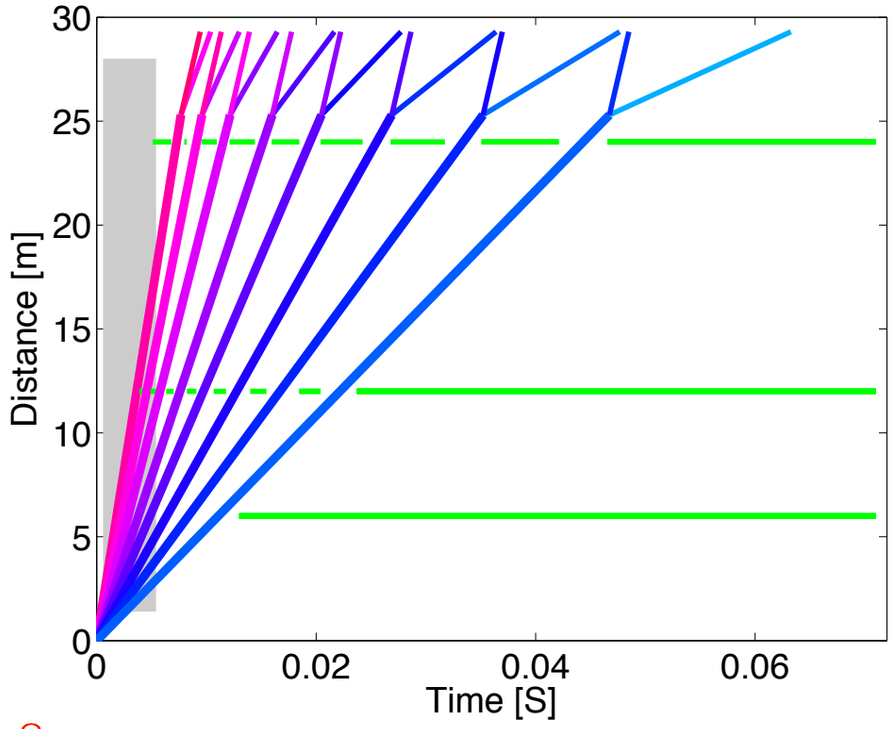




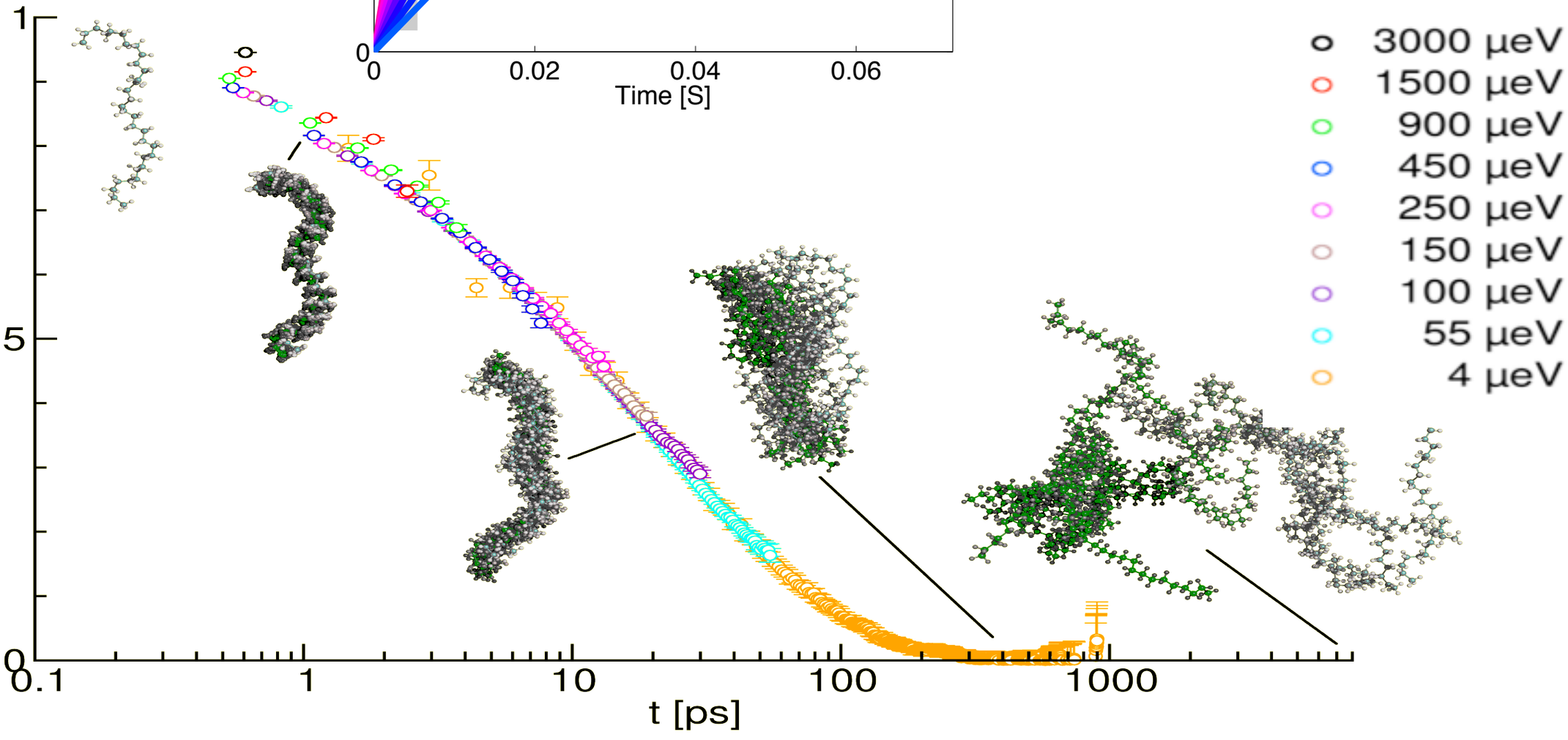
Down to 4 μeV (at 10 Å)

1 % ΔE/E @1 Å

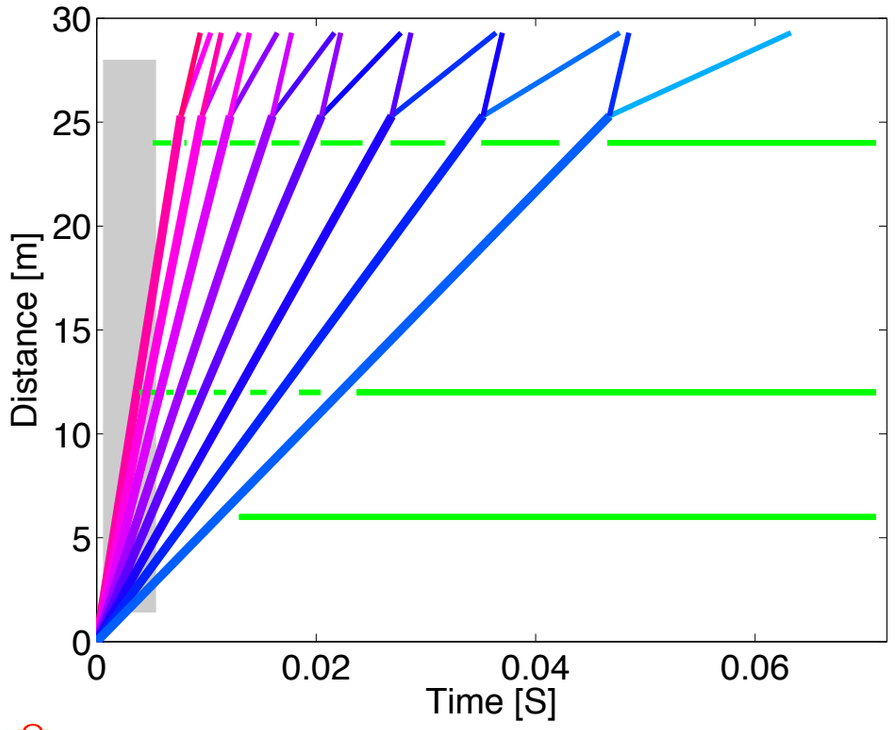
Repetition Rate Multiplication



TOFTOF: T. Unruh ~ 3 days

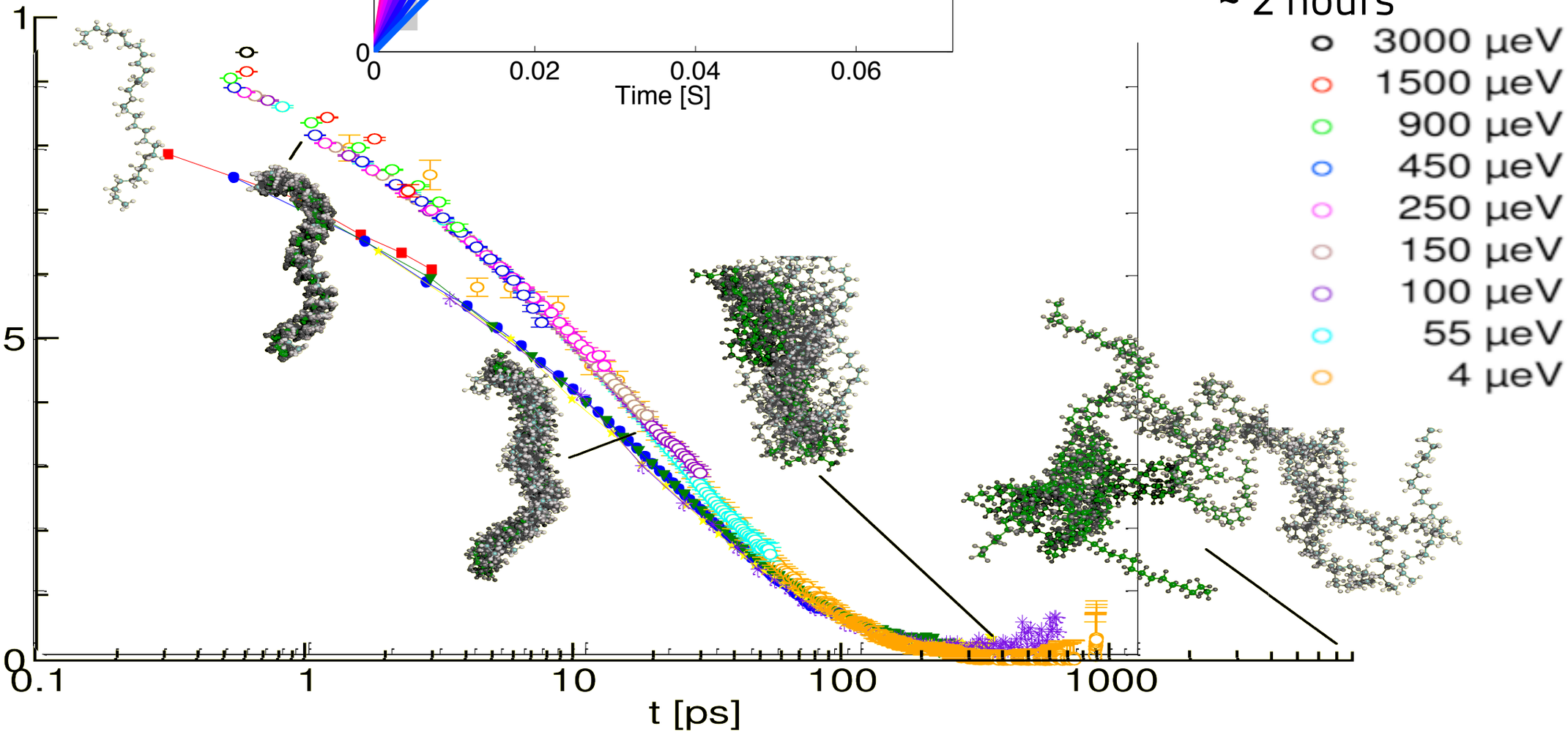


Repetition Rate Multiplication



TOFTOF: T. Unruh ~ 3 days

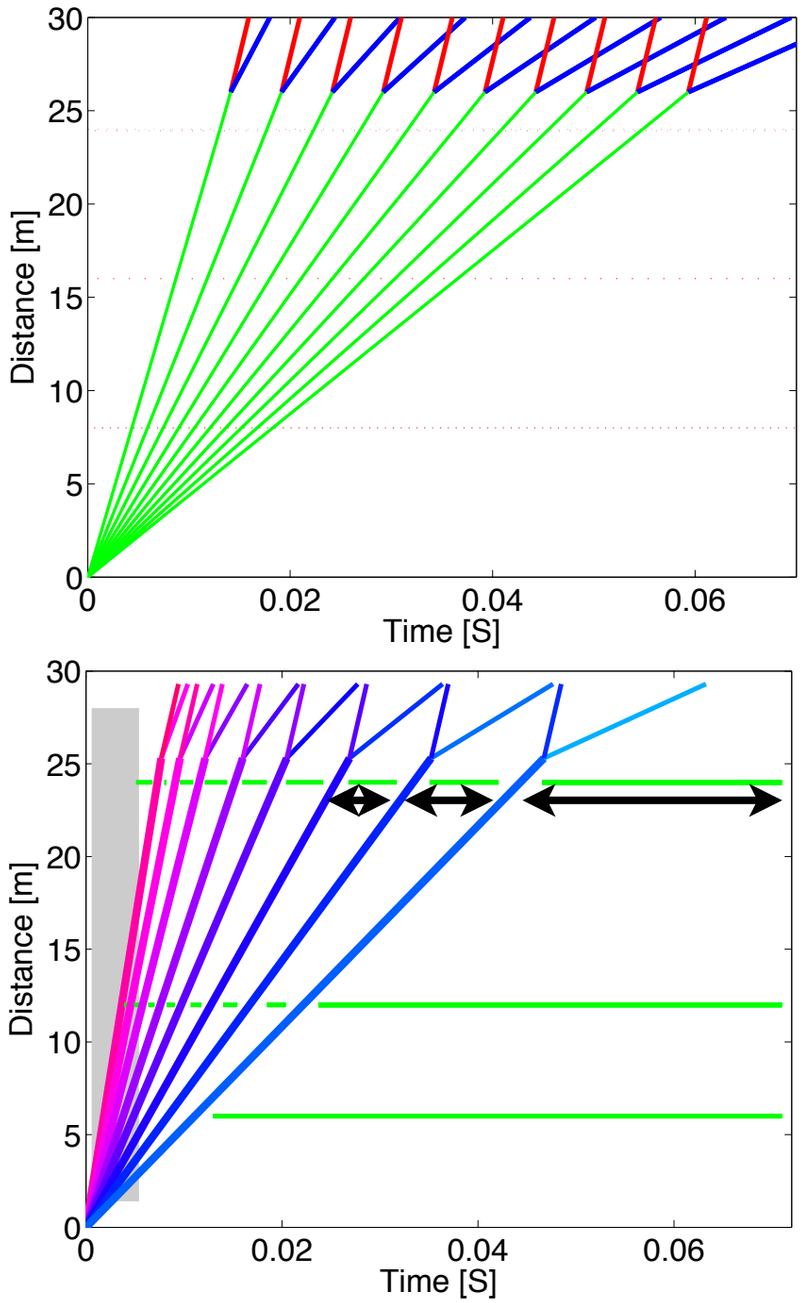
LET: P.P.Deen, R.Bewley
~ 2 hours



Repetition Rate Multiplication

Two issues to resolve:

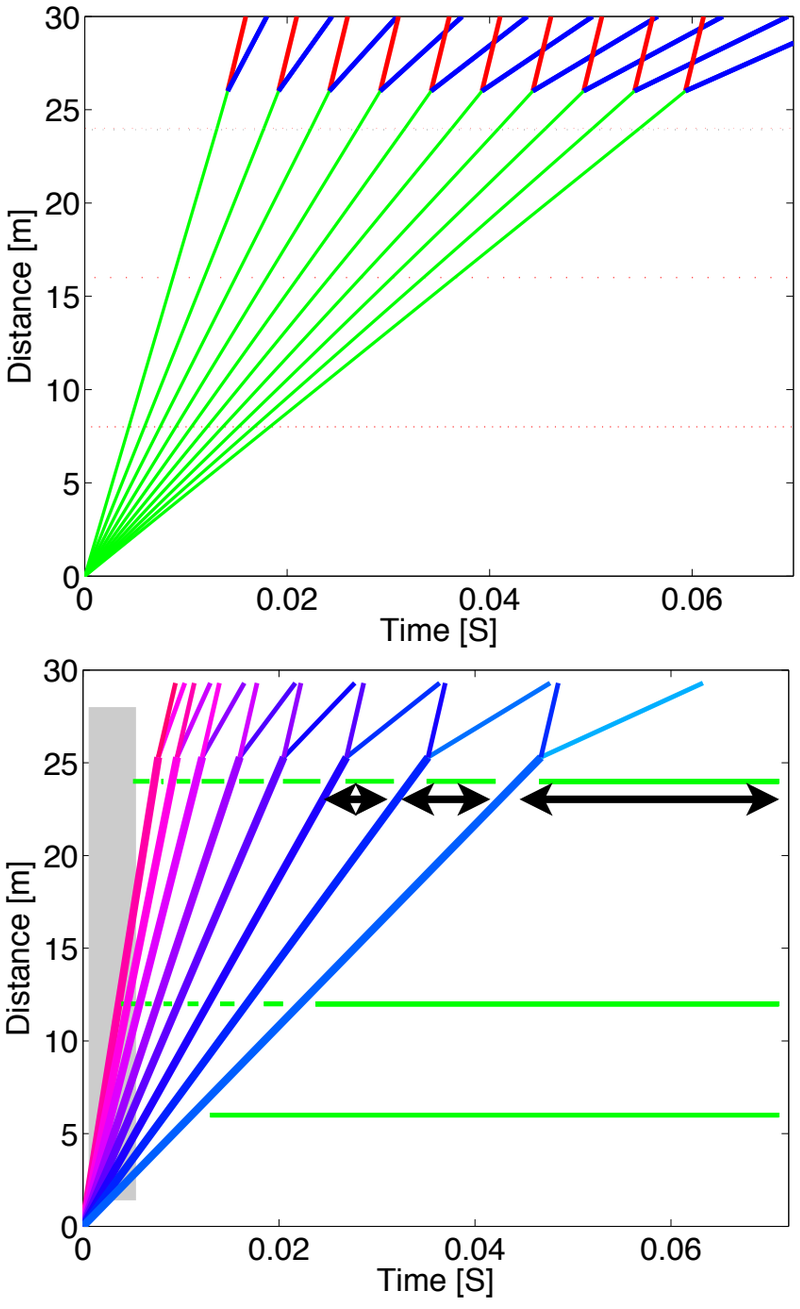
- Variable time between pulses (Access $E_F = 0.2\ E_i$ & $E_F = 250$ K)

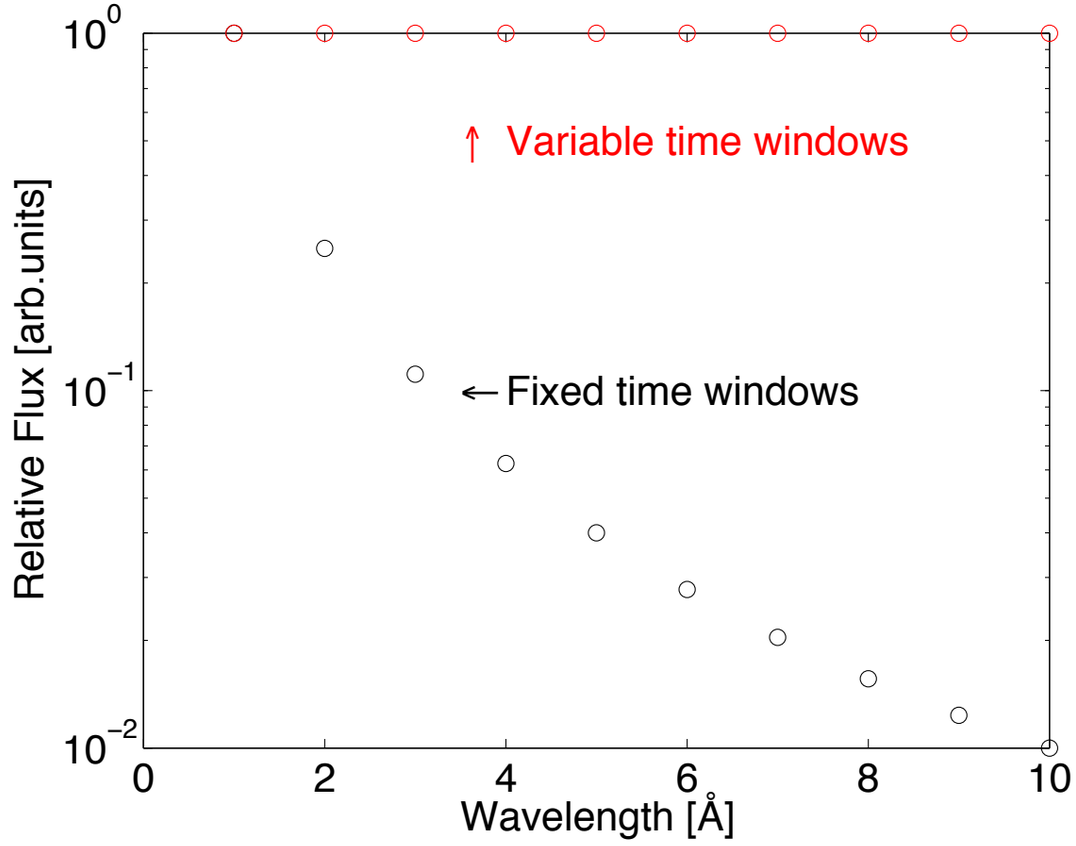


Repetition Rate Multiplication

Two issues to resolve:

- Variable time between pulses (Access $E_F = 0.2\ E_i$ & $E_F = 250$ K)
- Variable resolutions as a function of λ



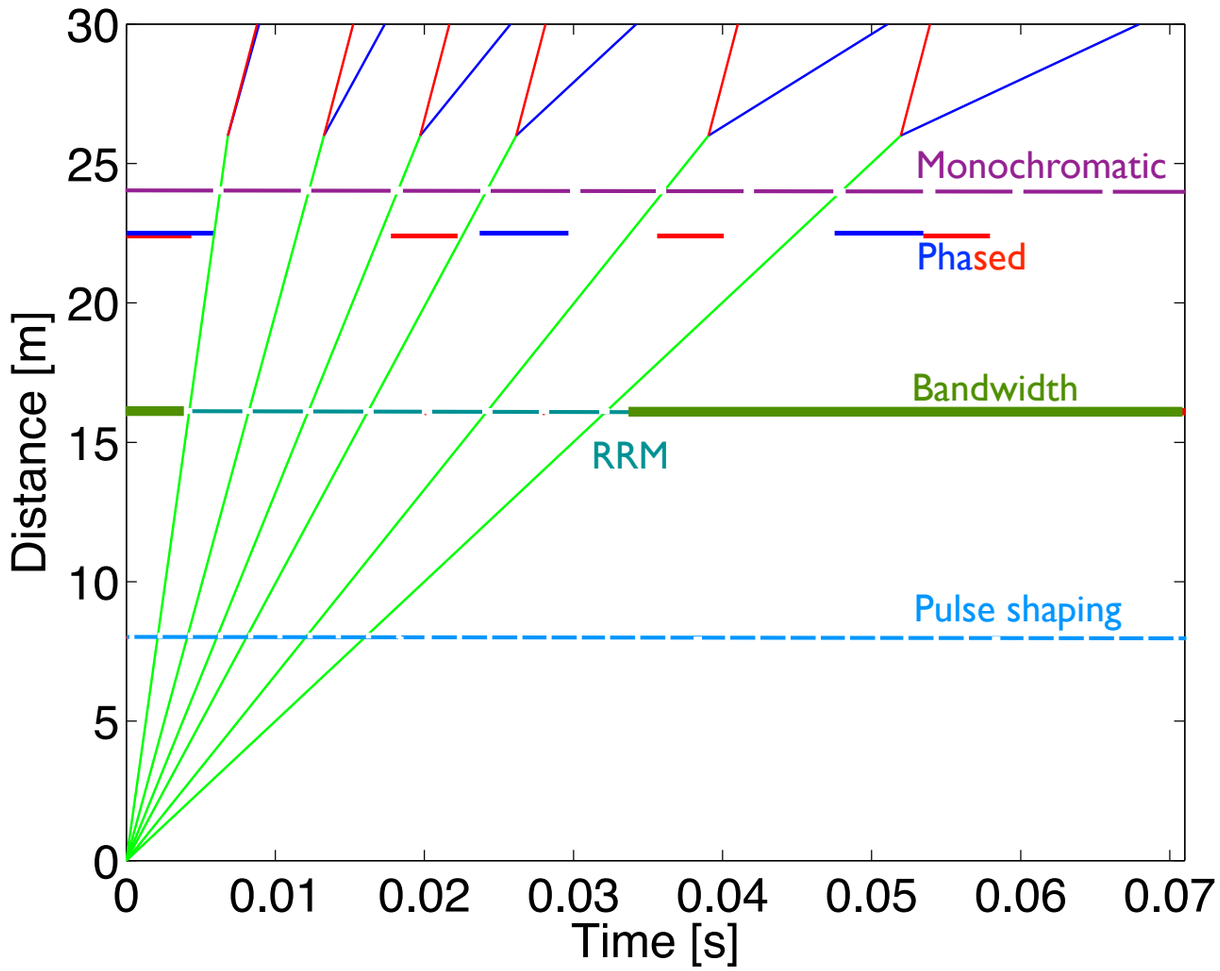


Repetition Rate Multiplication
Problem A
Out of phase choppers

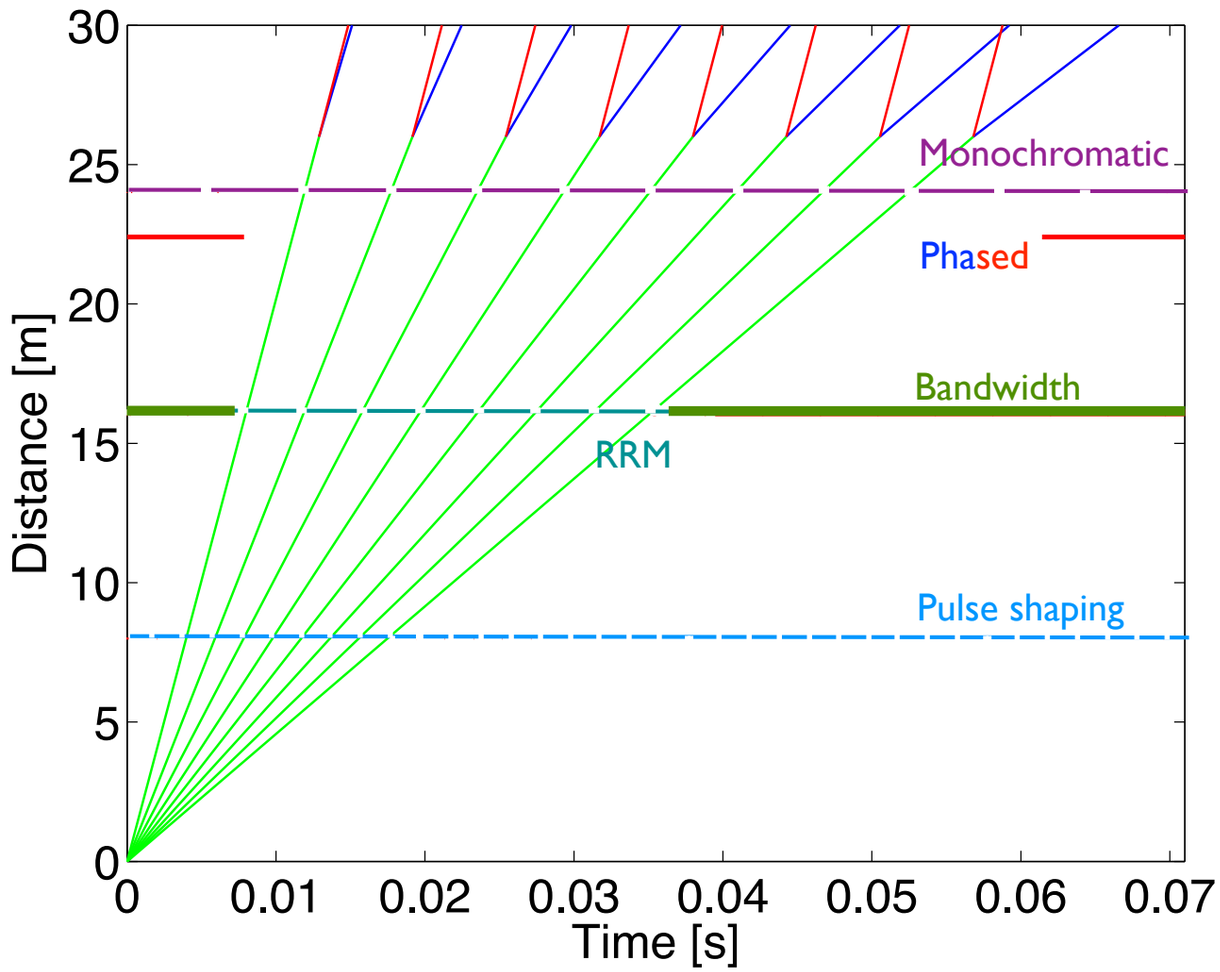
N*14 Hz

(N+1)*14 Hz

Inelastic scattering



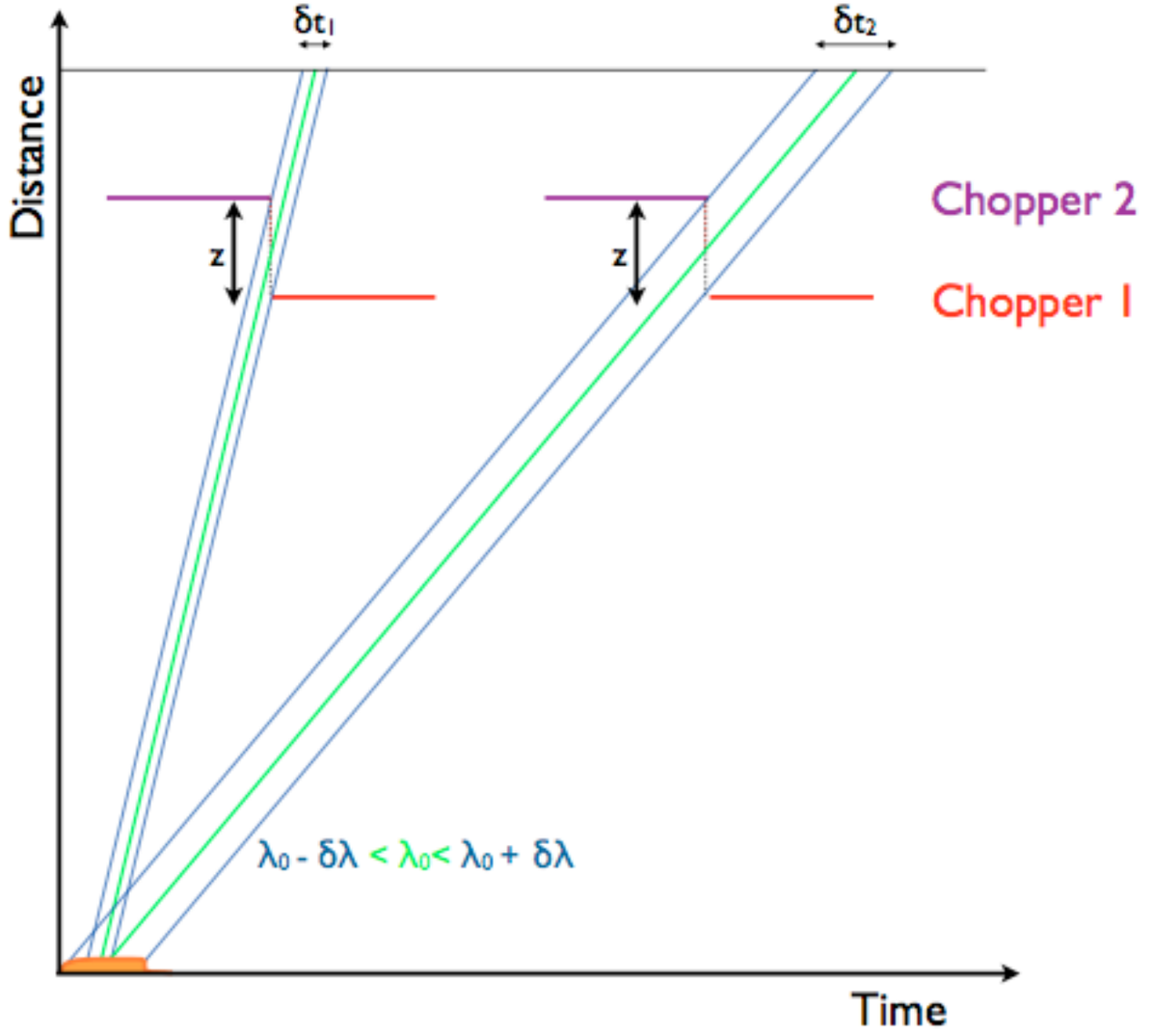
QES scattering



Variable time windows ✔

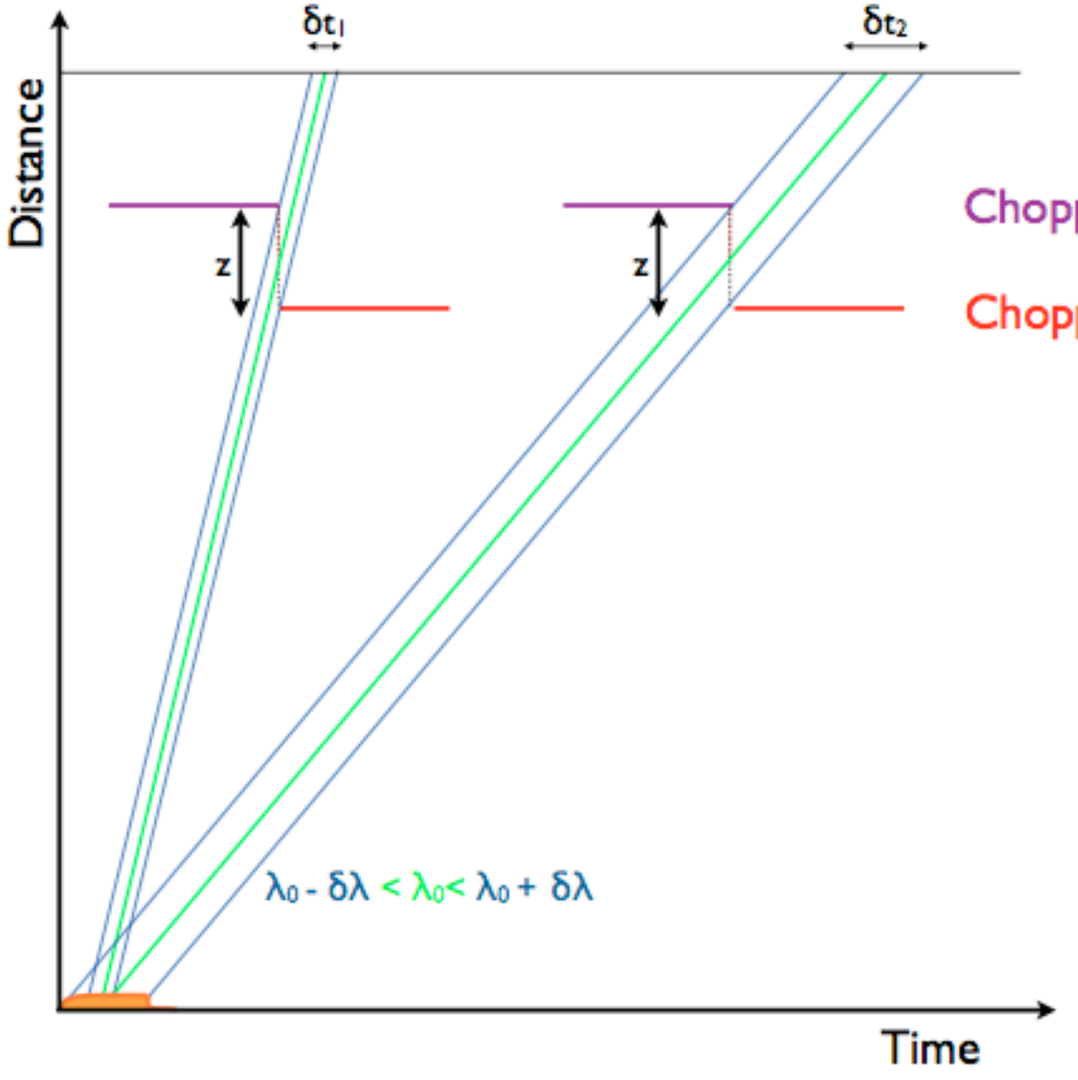
Repetition Rate Multiplication
Problem B

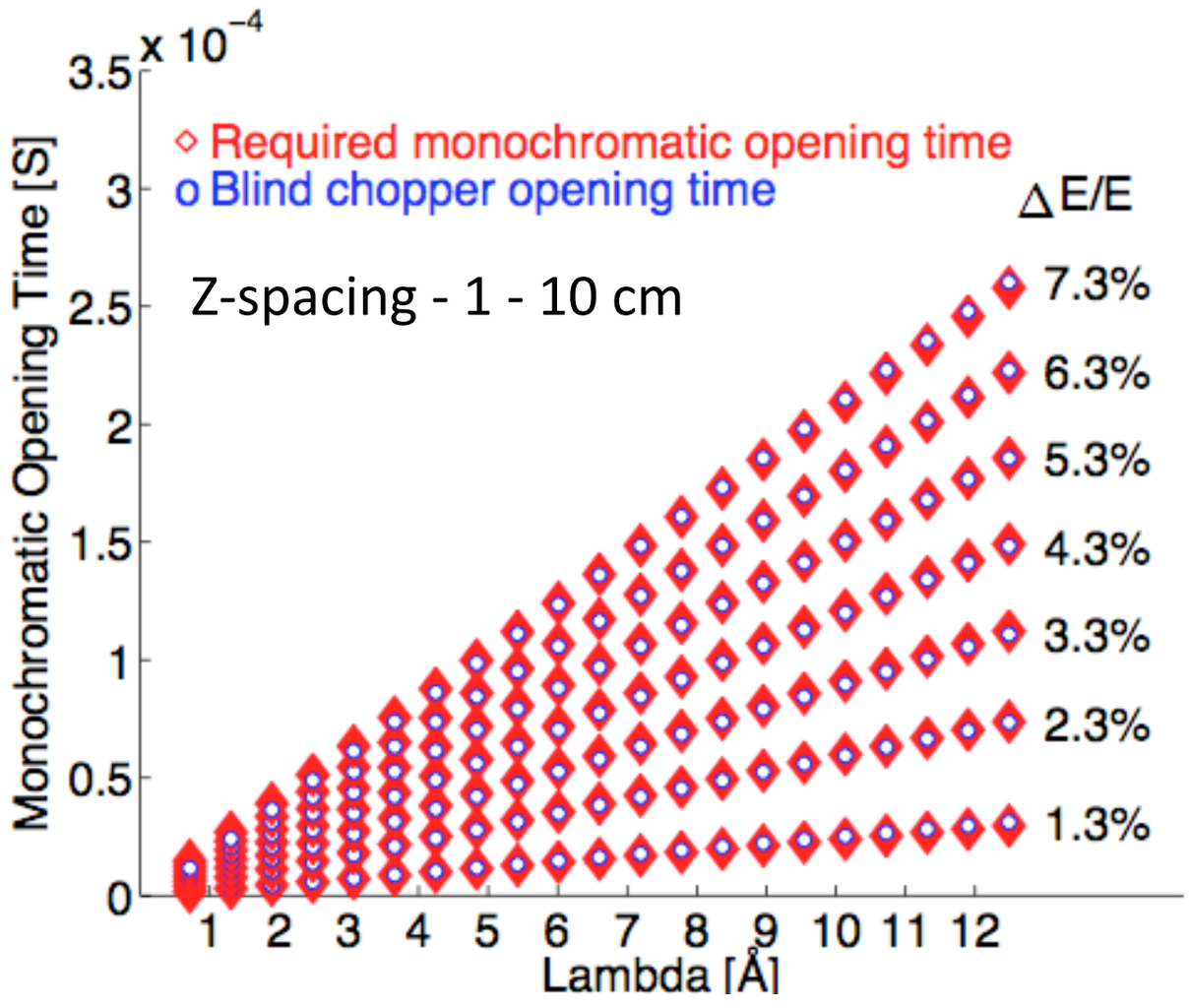
Analytically: Constant energy resolution



Repetition Rate Multiplication
Problem B

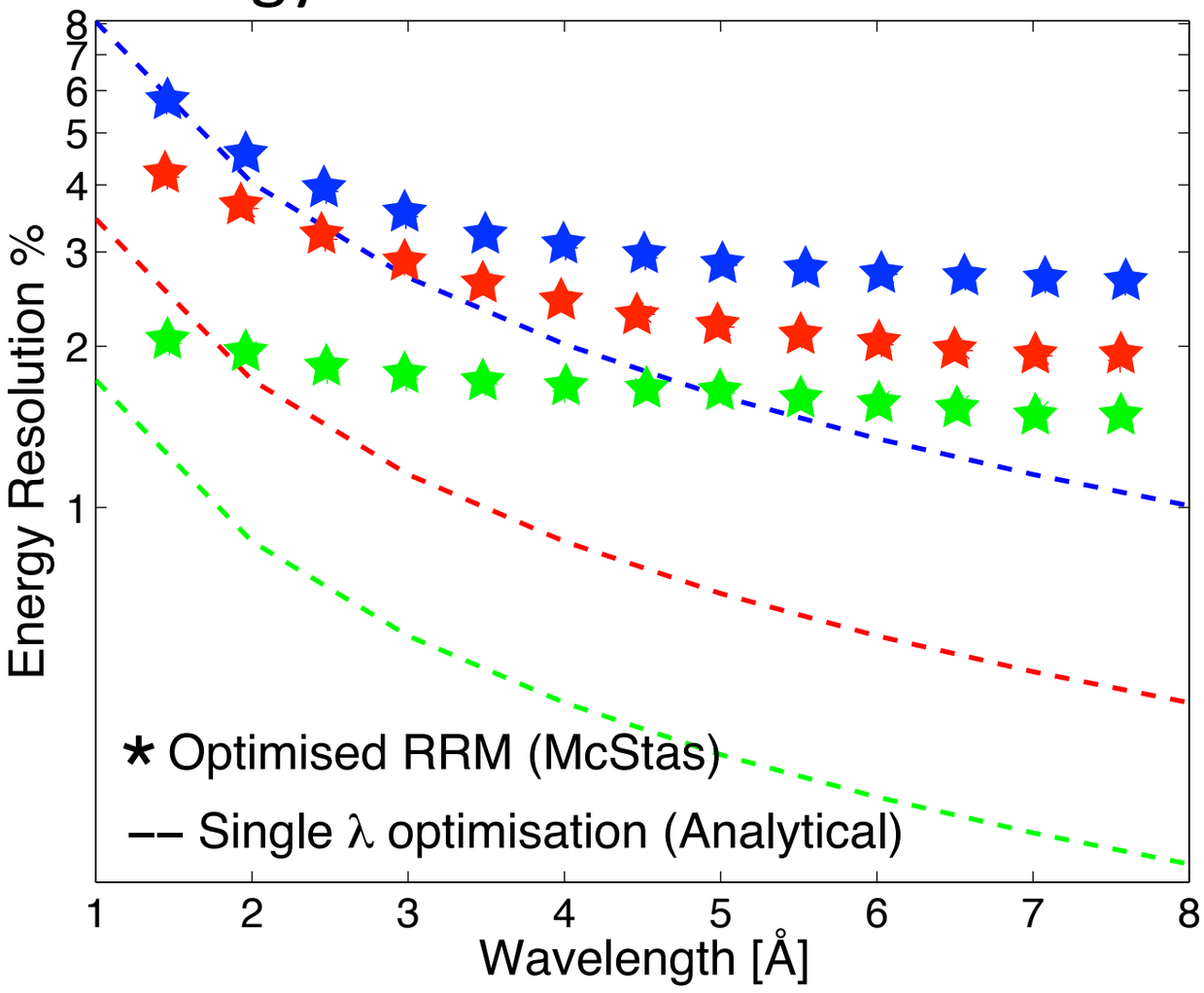
Analytically: Constant energy resolution





Repetition Rate Multiplication
Problem B

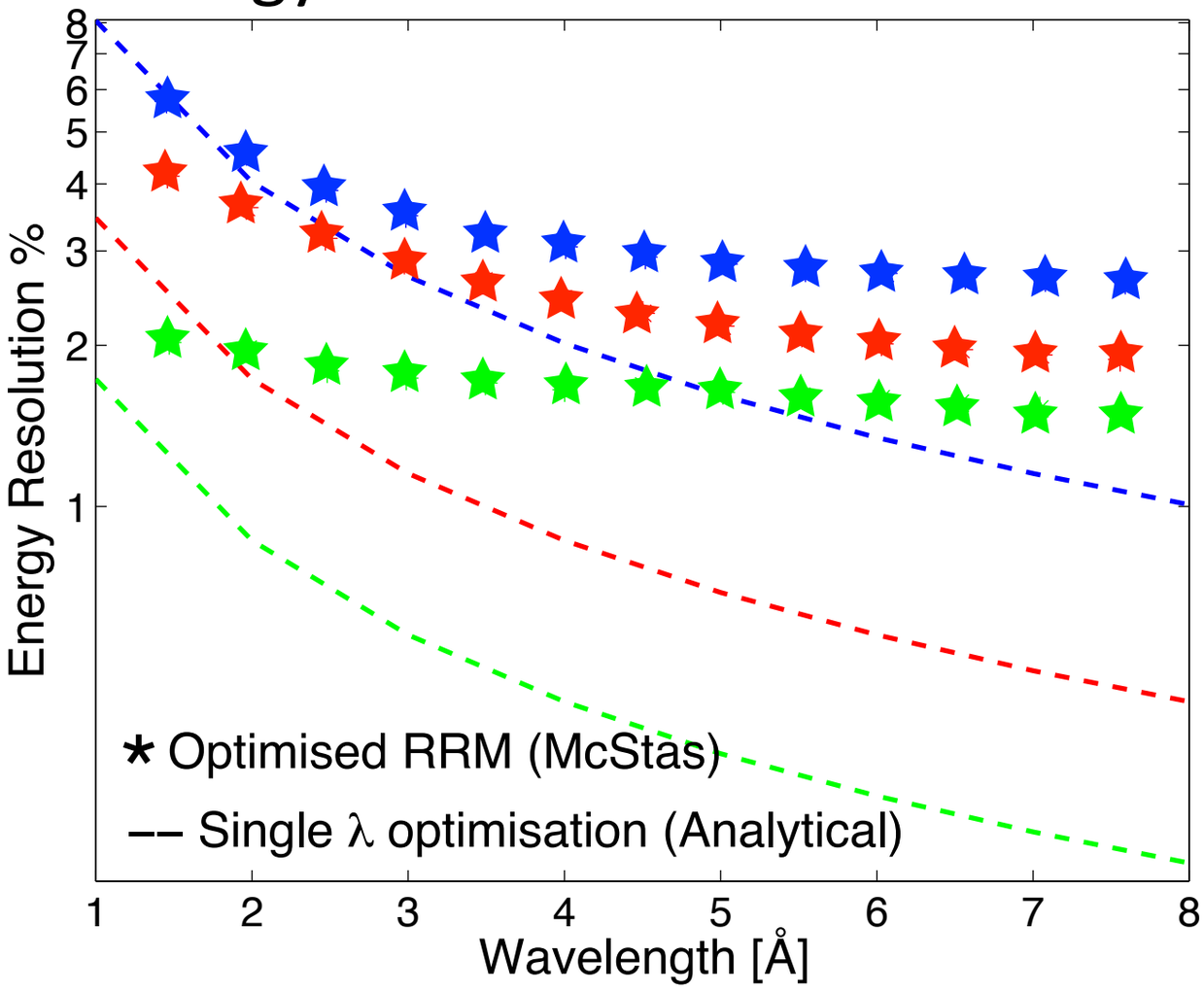
Energy Resolution



EUROPEAN SPALLATION SOURCE

Repetition Rate Multiplication Problem B

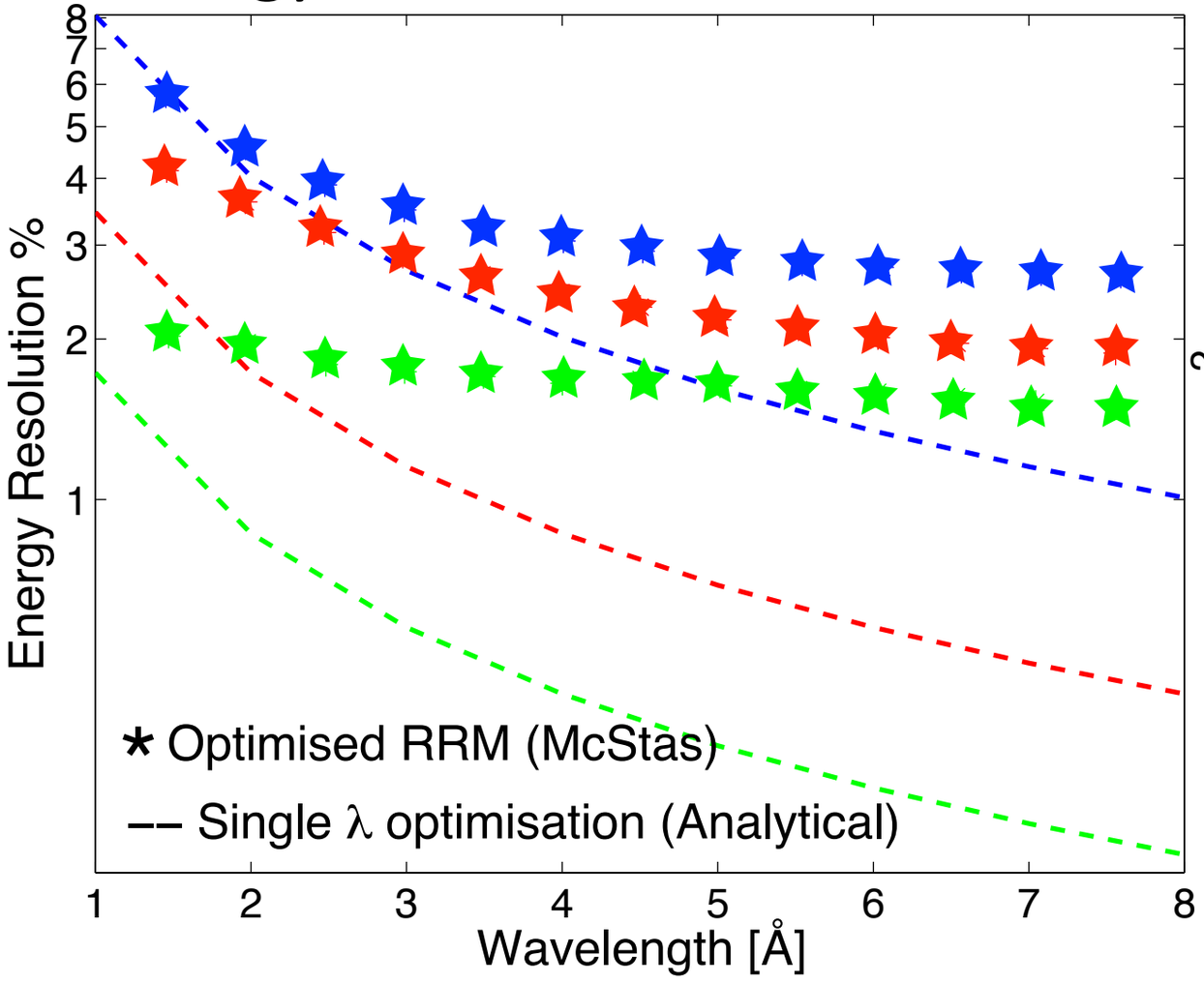
Energy Resolution



Constant energy resolution ✔

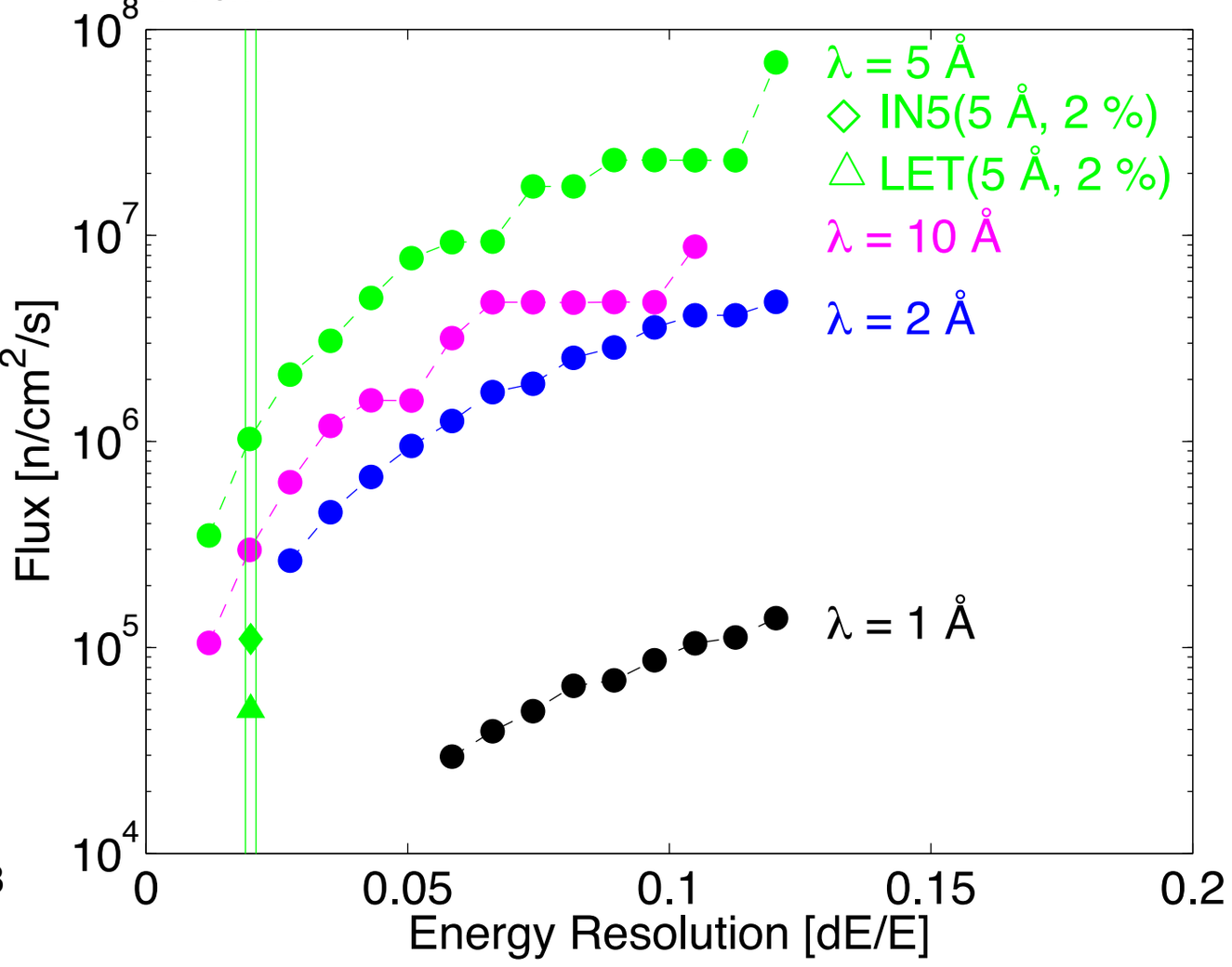
Repetition Rate Multiplication
Problem B

Energy Resolution



Constant energy resolution ✔

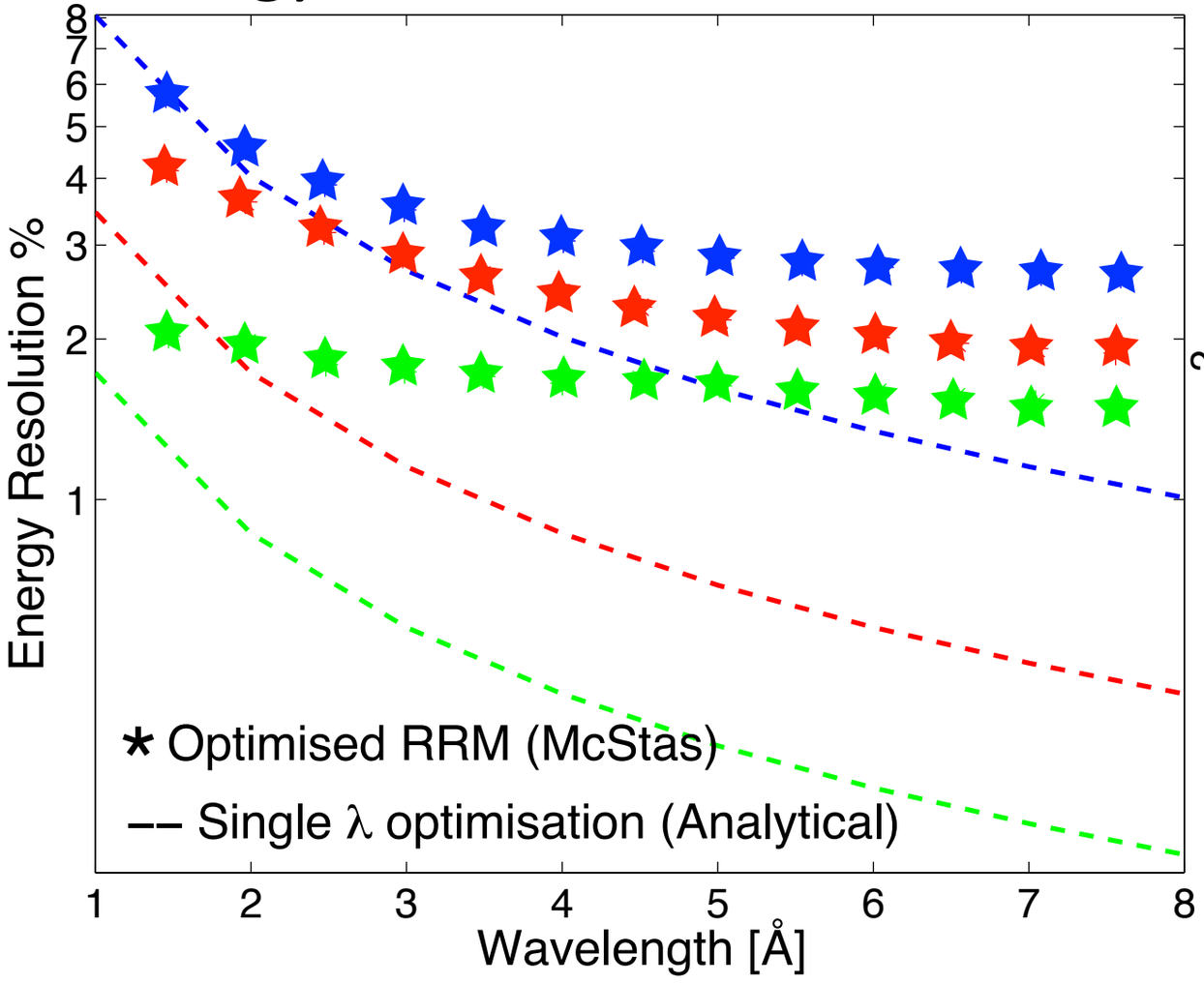
Flux



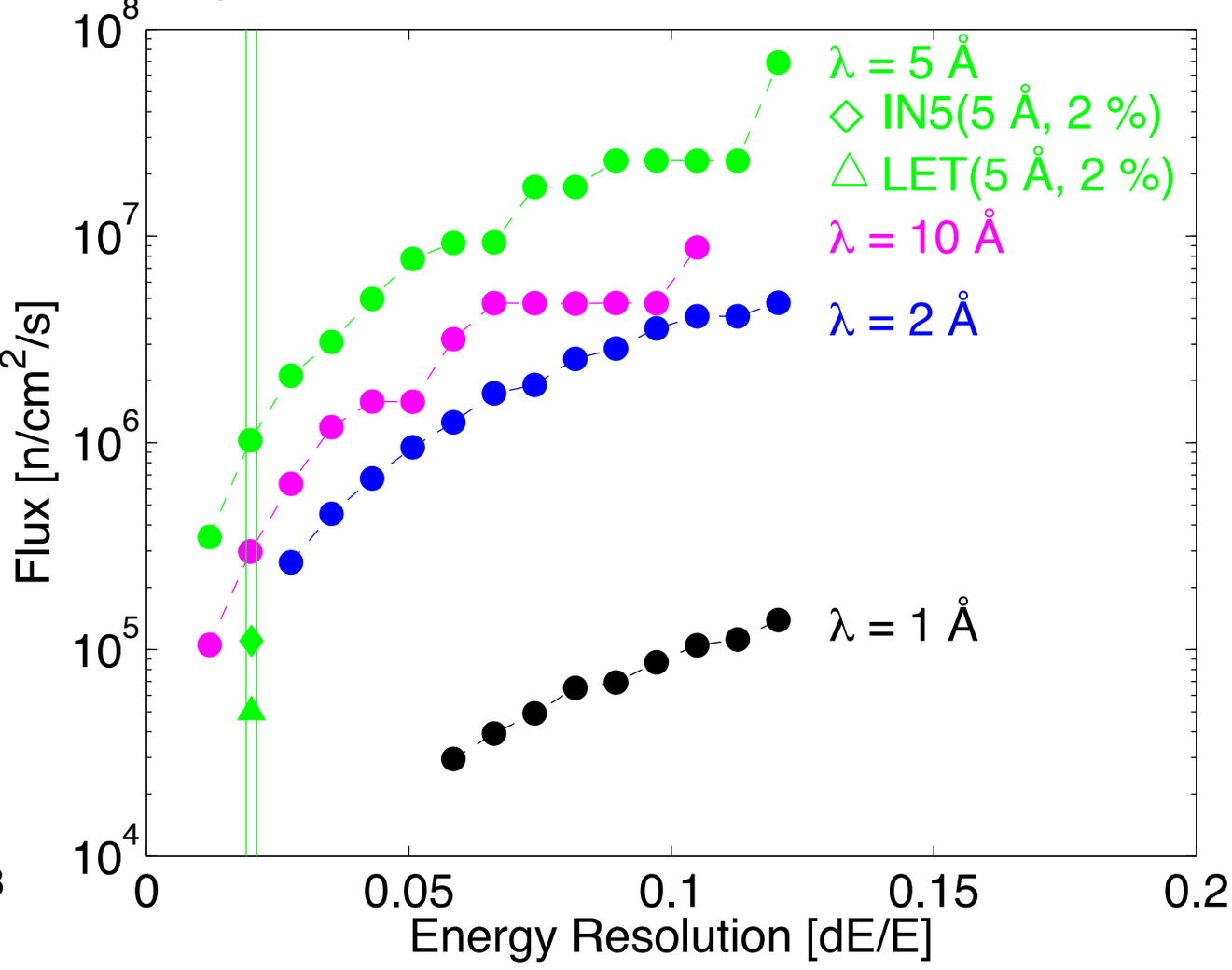
Tremendous flux gains ✔

Repetition Rate Multiplication
Problem B

Energy Resolution



Flux



Constant energy resolution ✔

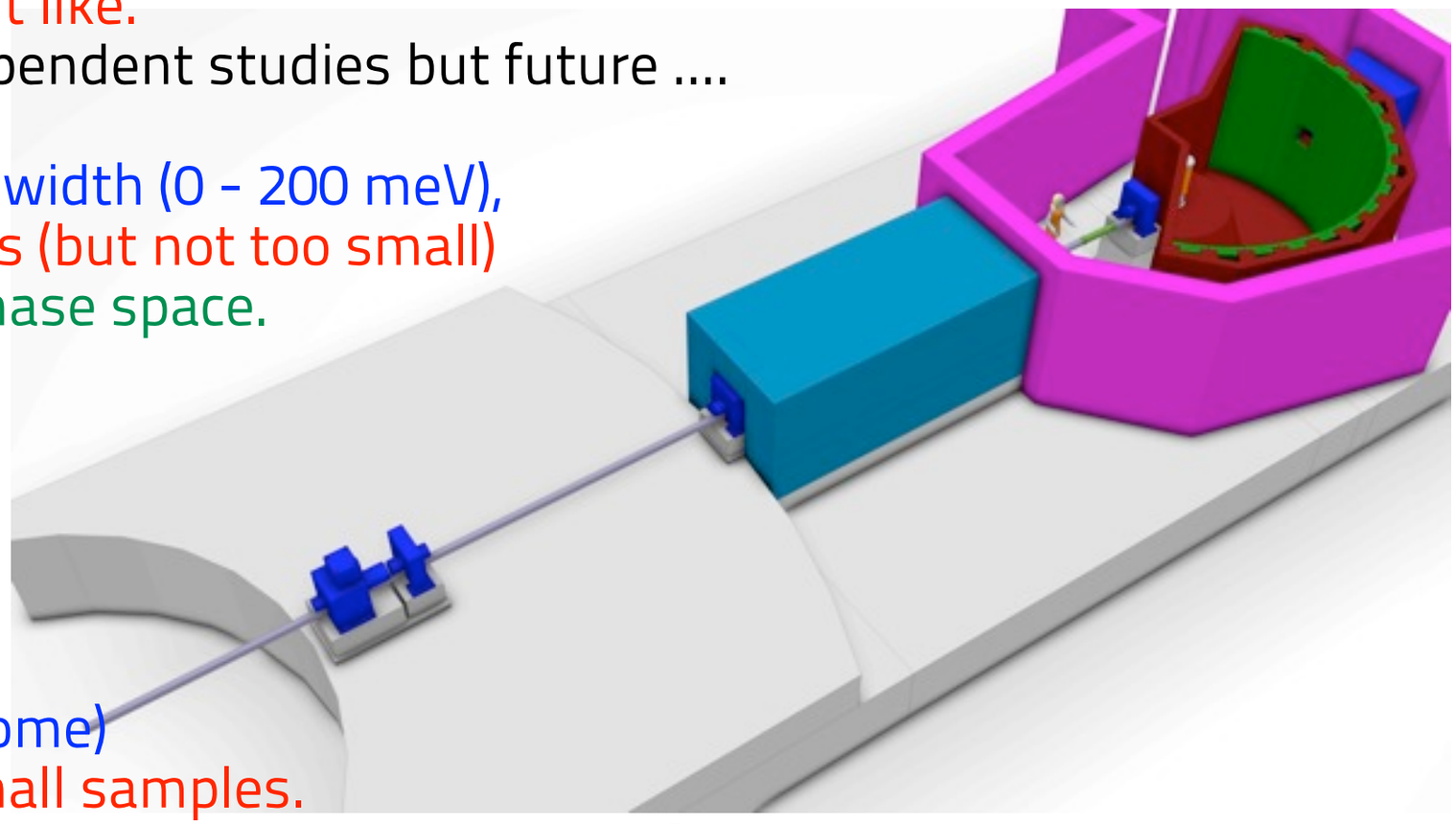
Tremendous flux gains ✔

Chopper spectrometer is fully optimised with RRM in mind

VOR - Wide bandwidth bispectral chopper spectrometer
Versatile Optimal Resolution chopper spectrometer

Soft matter: Broad bandwidth
Variable energy resolution (several μeV - 3000 μeV)
Be able to relax resolution for weak scattering signals
Availability of high momentum transfer (Q < 11 Angstrom)
High flux but not necessarily point like.
Currently limited number of Q dependent studies but future ....

Functional materials: Broad bandwidth (0 - 200 meV),
Clean/limited and flat flux profiles (but not too small)
High flux (x 10 - 100) probe (P) phase space.
High resolution at high energies.



Magnetism: Broad bandwidth (some)
Flux focussed on small samples.
Q-dependence important, clean divergence profiles
High energy resolution - ΔE/E ~ 1-3%

Gas Storage & Catalysis: Broad bandwidth
In-operando studies (second)
Small samples but not point like.
Two orders of magnitude in flux

VOR - Wide bandwidth bispectral chopper spectrometer
Versatile Optimal Resolution chopper spectrometer

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Variable energy resolution (several μeV - 3000 μeV)
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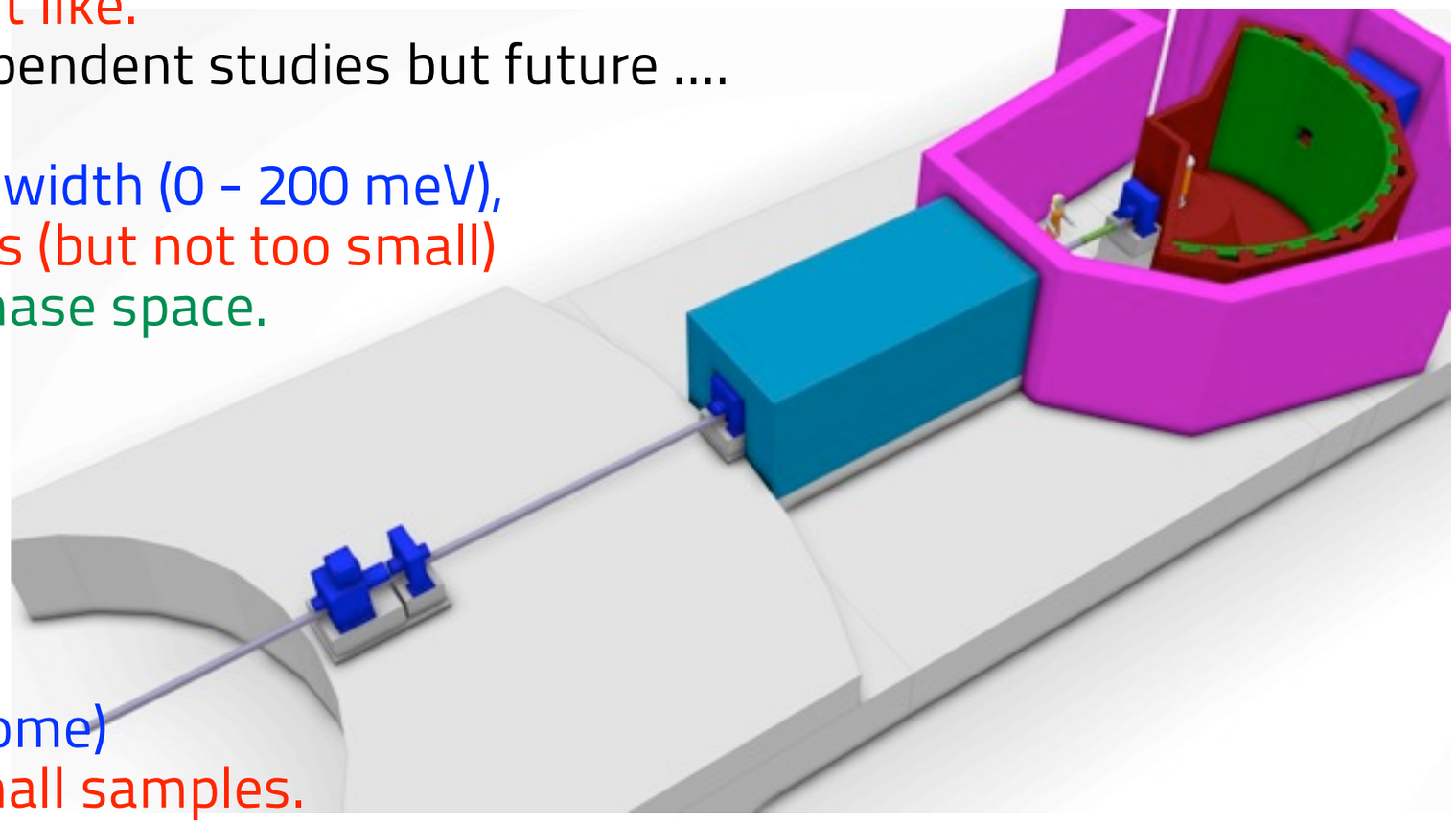
Detectors
See R. H. Wilton



Functional materials: Broad bandwidth (0 - 200 meV),
Clean/limited and flat flux profiles (but not too small)
High flux (x 10 - 100) probe (P) phase space.
High resolution at high energies.

Magnetism: Broad bandwidth (some)
Flux focussed on small samples.
Q-dependence important, clean divergence profiles
High energy resolution - ΔE/E ~ 1-3%

Gas Storage & Catalysis: Broad bandwidth
In-operando studies (second)
Small samples but not point like.
Two orders of magnitude in flux

VOR
Versatile Optimal Resolution chopper spectrometer

VOR
Goddess who knows all

New scientific avenues.
Answer open questions.
Create many new ones.

IKON 25 - 26th September

EUROPEAN SPALLATION SOURCE

Pascale P. Deen
Anette Vickery

EUROPEAN
SPALLATION
SOURCE