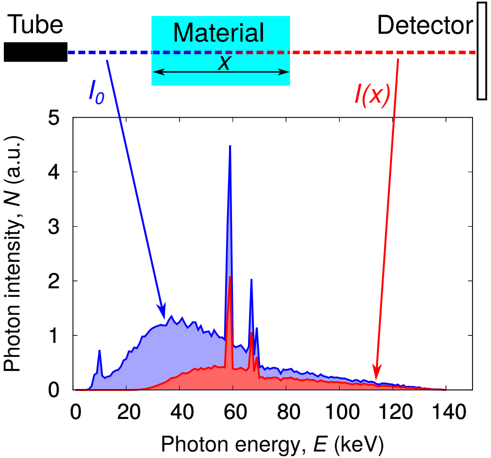
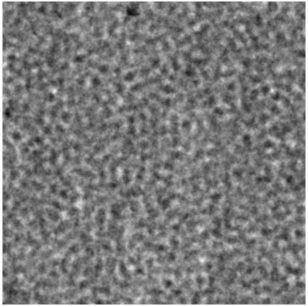
X-ray radiography of granular systems – particle densities and dynamics





FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

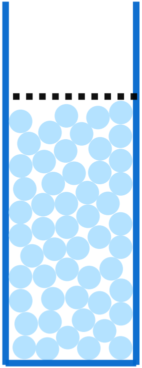
Institute for Multiscale Simulation MSS

PhD defense

Manuel Baur

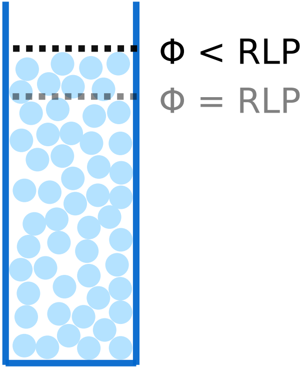
Funded by the German Federal Ministry for Economic Affairs and Energy, grant no. 50WM 1653

X-ray radiography of granular systems – particle densities and dynamics



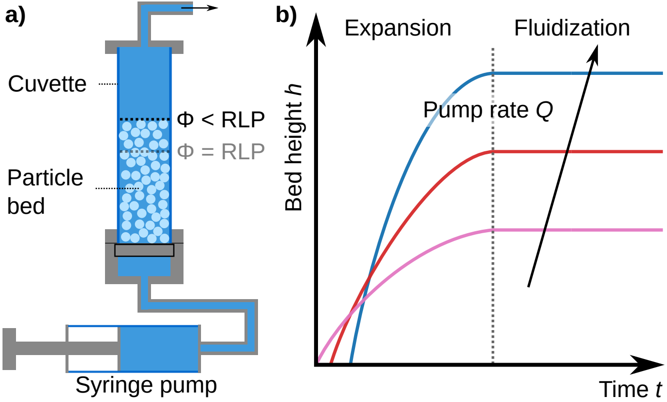
Φ = RLP

X-ray radiography of granular systems – particle densities and dynamics



X-ray radiography of granular systems – particle densities and dynamics

Fluidized bed



X-ray radiography of granular systems – particle densities and dynamics

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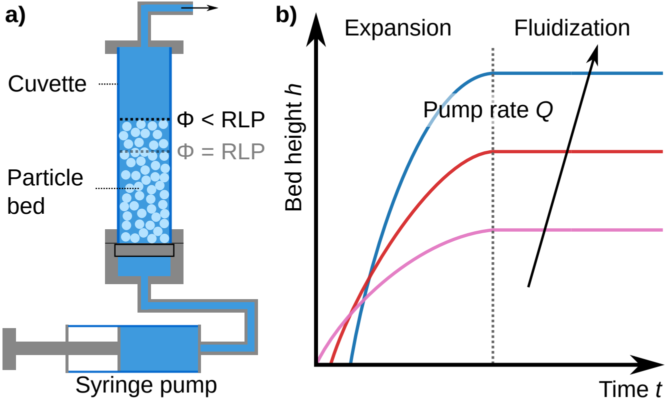
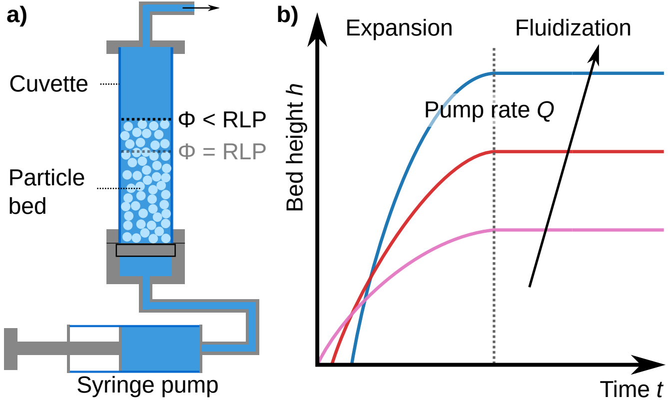


X-ray radiography of granular systems – particle densities and dynamics

Densities

Dynamics

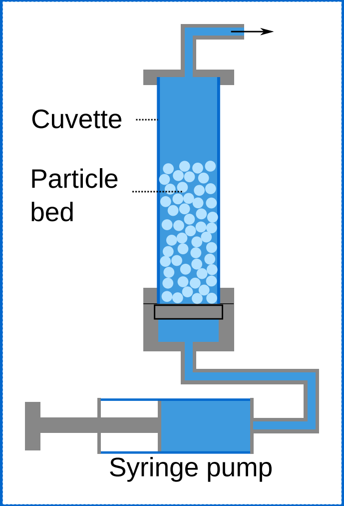
Fluidized bed

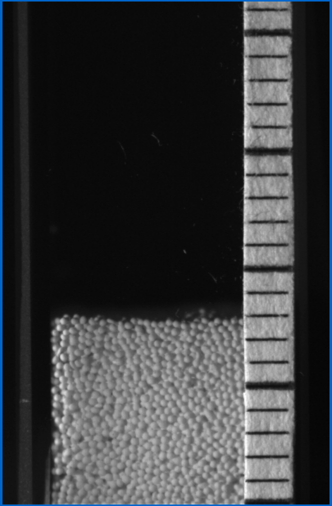


Fluidized bed reactor

"**Lack of understanding:**
It is very difficult to predict and calculate the complex mass [...] flows within the bed."

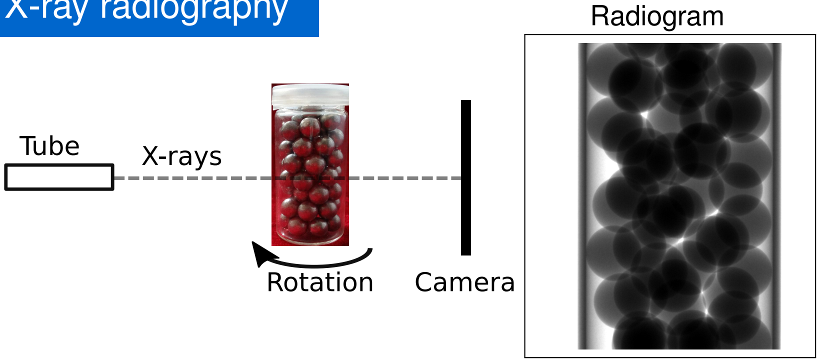
Particulate flows are **opaque**





Master thesis Welm Pätzold

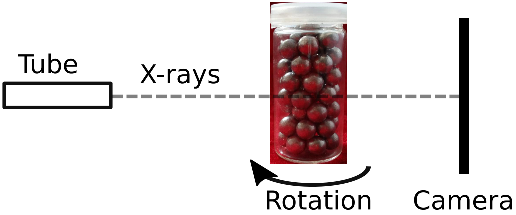
X-ray radiography



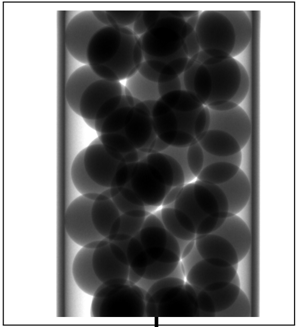
2D projections of 3D object

Short acquisition time

X-ray radiography



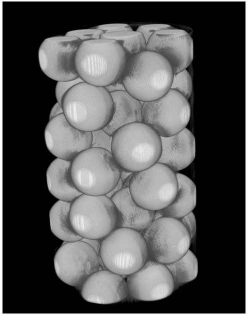
Radiogram



2D projections of 3D object
Short acquisition time

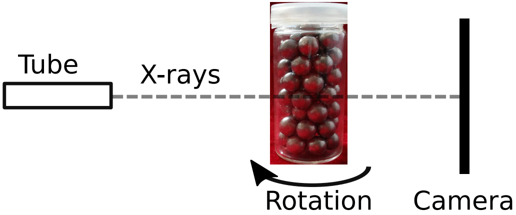
Reconstruction from
800 projections

Tomogram

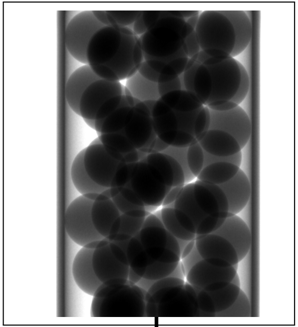


Full 3D information
Long acquisition time
→ static objects

X-ray radiography



Radiogram



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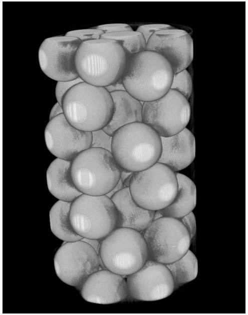
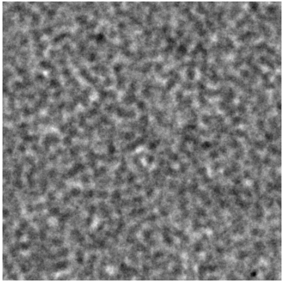


Full 3D information

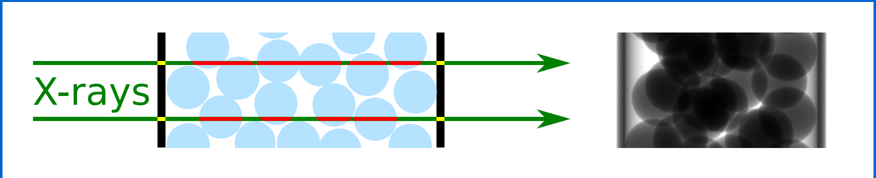
Long acquisition time

→ static objects

Dynamic system



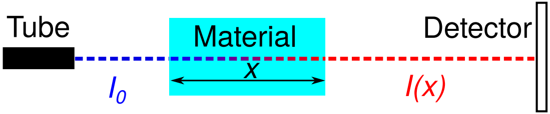
Measuring the volume fraction of **dynamic** granular systems



Correction of beam hardening in X-ray radiograms

Baur *et al*, *Rev. Sci. Instrum.* (2019)
In collaboration with Norman Uhlmann, Fraunhofer EZRT

Attenuation of X-rays

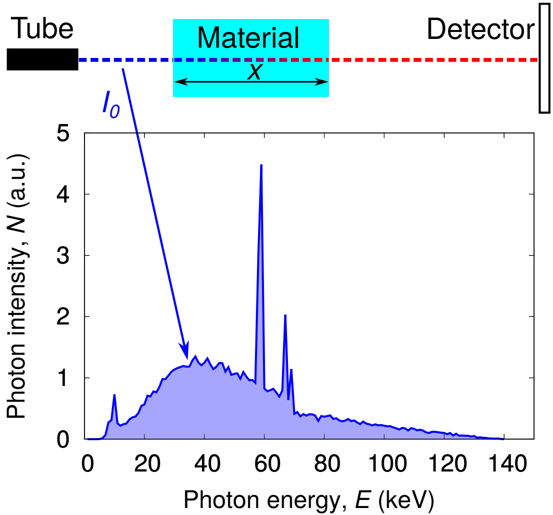


Beer-Lambert's law

$$I(x) = I_0 \exp(-\mu x)$$

Thickness: $x = -\frac{1}{\mu} \ln \frac{I(x)}{I_0}$

Attenuation of X-rays

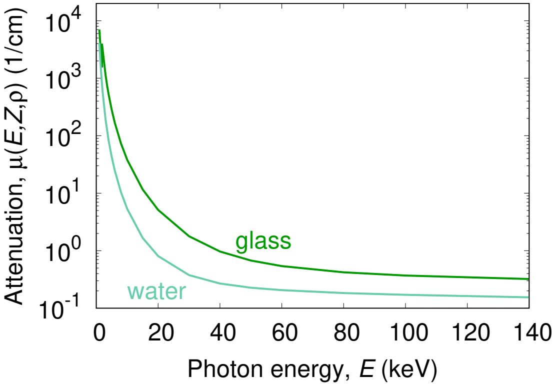


Beer-Lambert's law

$\mu \neq \text{const}$

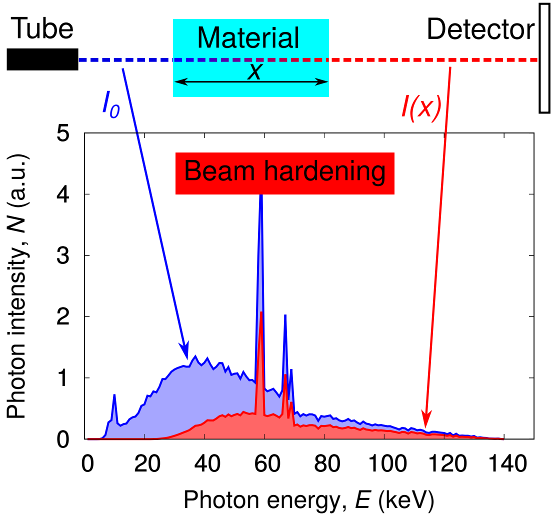
$$I(x) = I_0 \exp(-\mu(E, Z, \rho)\, x)$$

Thickness: $x = ?$



`https://www.nist.gov/pml/x-ray-mass-attenuation-coefficients`

Attenuation of X-rays



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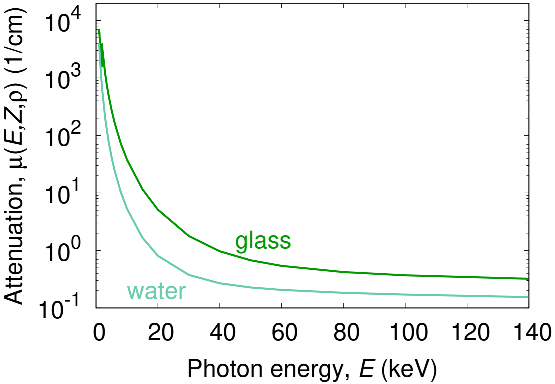
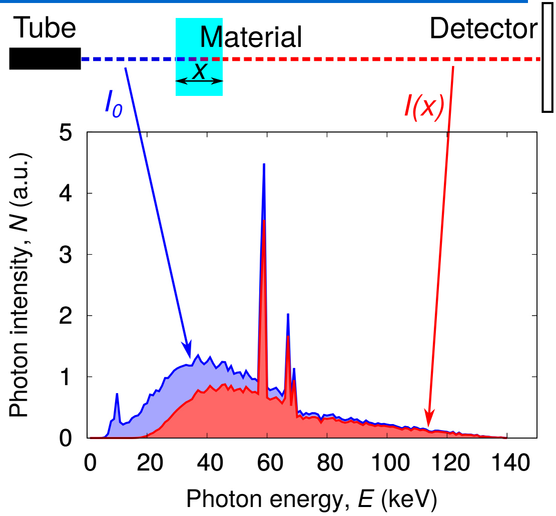
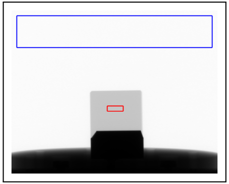


`https://www.nist.gov/pml/x-ray-mass-attenuation-coefficients`

The effective attenuation, $\mu_{\text{eff}}(x)$

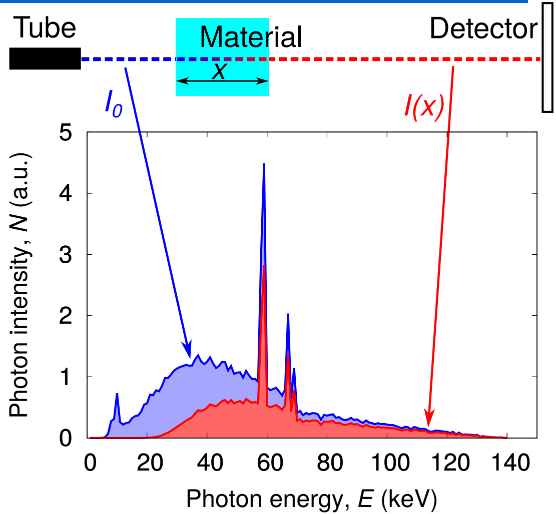


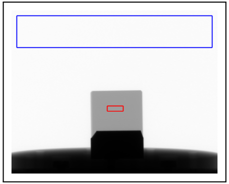


effective attenuation:

$$I(x) = I_0 \exp(-\mu_{\text{eff}}(x)\, x)$$

The effective attenuation, $\mu_{\text{eff}}(x)$





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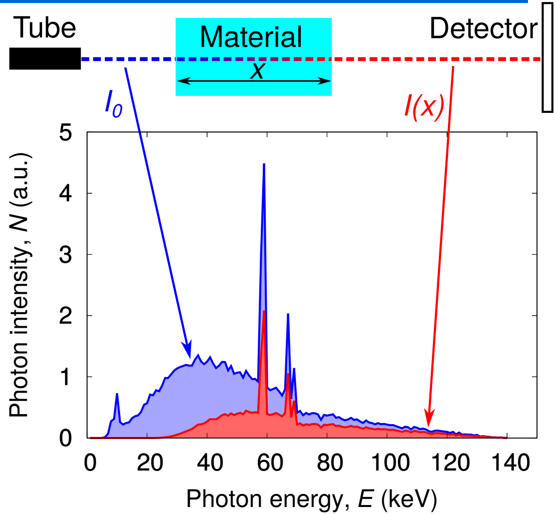
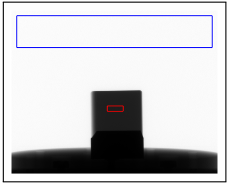
The effective attenuation, $\mu_{\text{eff}}(x)$

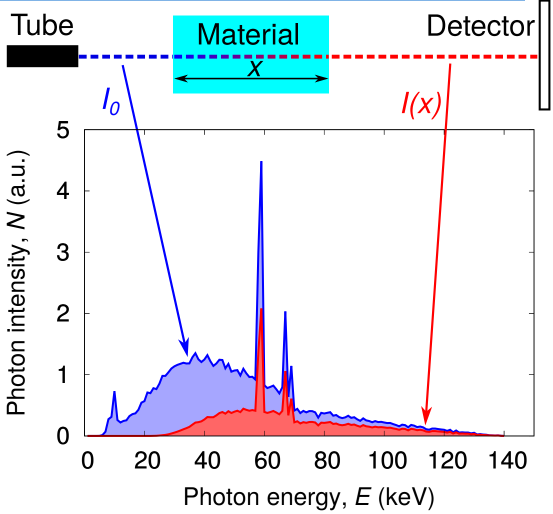


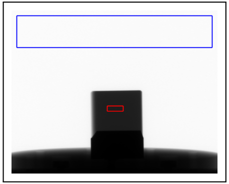


effective attenuation:

$$I(x) = I_0 \exp(-\mu_{\text{eff}}(x)\, x)$$

The effective attenuation, $\mu_{\text{eff}}(x)$

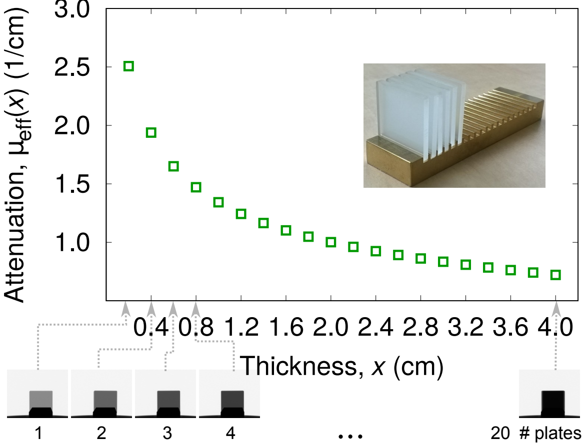




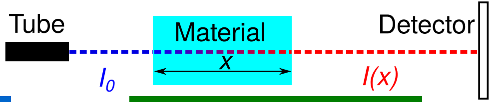
effective attenuation:

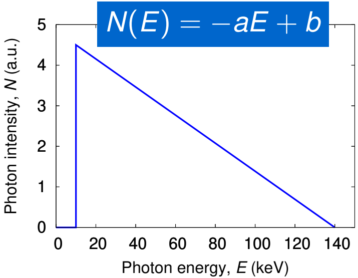
$$I(x) = I_0 \exp(-\mu_{\text{eff}}(x)\, x)$$

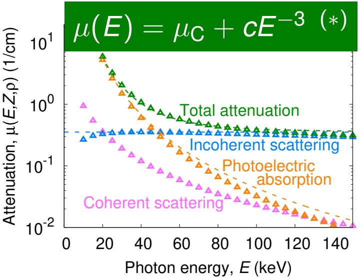
$$\mu_{\text{eff}}(x) = -\frac{1}{x} \frac{I(x)}{I_0}$$

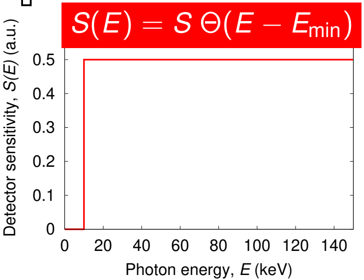


Modeling of $\mu_{\text{eff}}(x)$





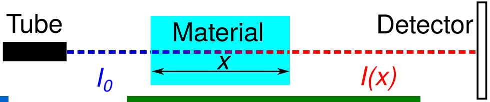




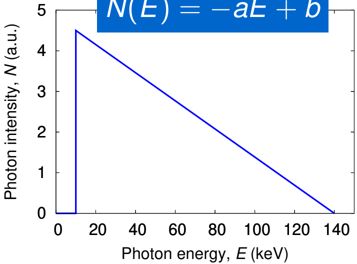
$$I(x) \propto \int N(E)\, \exp\{-\mu(E, Z, \rho)x\}\, S(E)\, \mathrm{d}E$$

(∗) XCOM supplied by NIST

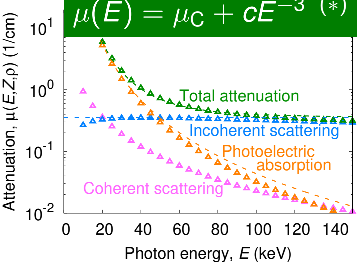
Modeling of $\mu_{\mathrm{eff}}(x)$



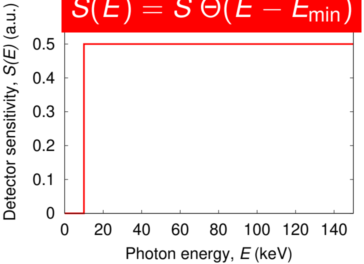
$$N(E) = -aE + b$$



$$\mu(E) = \mu_{\mathrm{C}} + cE^{-3} \quad (*)$$

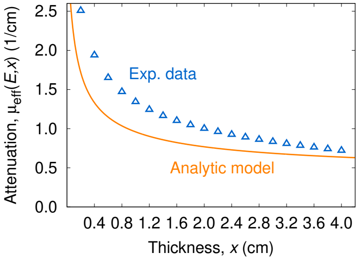


$$S(E) = S\,\Theta(E - E_{\mathrm{min}})$$



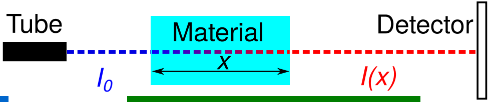
$$I(x) \propto \int N(E)\exp\{-\mu(E,Z,\rho)x\}S(E)\,\mathrm{d}E$$

$$\propto S\int_{E_{\mathrm{min}}}^{E_{\mathrm{max}}}(-aE+b)\exp\{-(\mu_{\mathrm{C}}+cE^{-3})x\}\mathrm{d}E$$

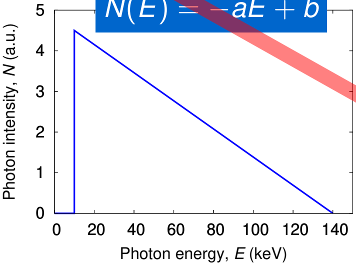


(∗) XCOM supplied by NIST

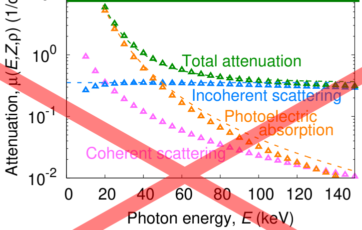
Modeling of $\mu_{\mathrm{eff}}(x)$



$$N(E) = -aE + b$$



$$\mu(E) = \mu_C + cE^{-3} \quad (*)$$



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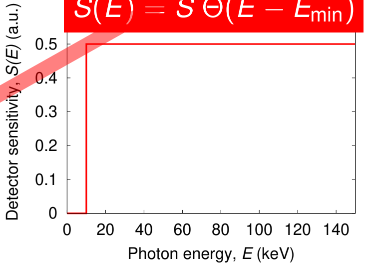

$$I(x) \propto \int N(E)\exp\{-\mu(E,Z,\rho)x\}S(E)\,\mathrm{d}E$$

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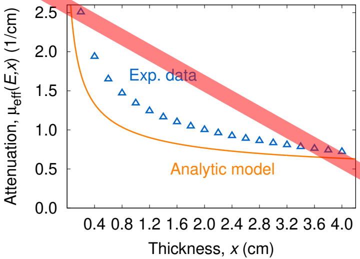
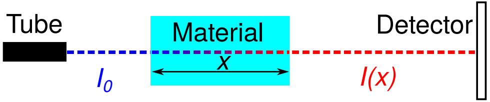
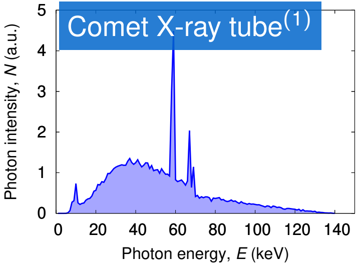
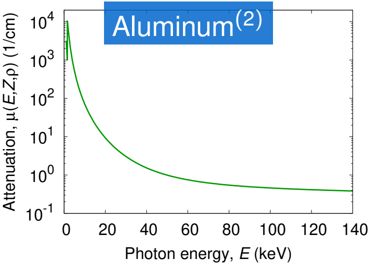


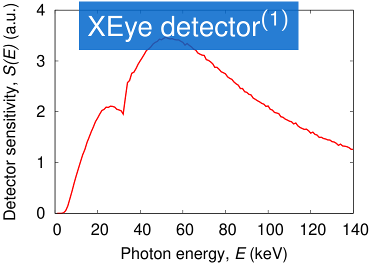
$(*)$ XCOM supplied by NIST

Numerical approx. of $\mu_{\mathrm{eff}}(x)$









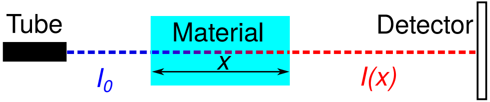
$$I(x) \propto \int N(E) \exp\{-\mu(E, Z, \rho)x\} S(E)\, \mathrm{d}E$$

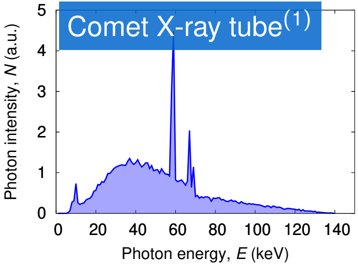
$$\int \rightarrow \sum$$

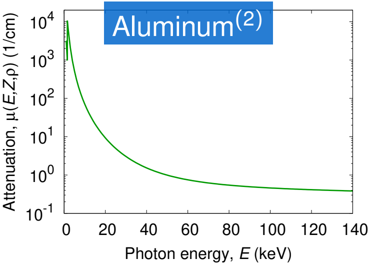
(1) Supplied by Norman Uhlmann, Fraunhofer EZRT

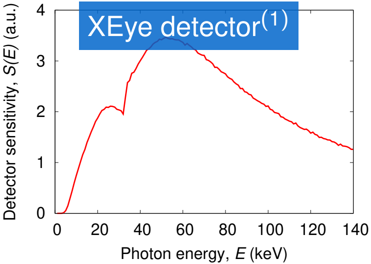
(2) XCOM supplied by NIST

Numerical approx. of $\mu_{\mathrm{eff}}(x)$









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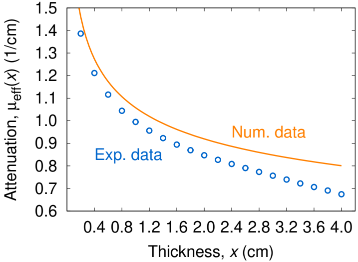
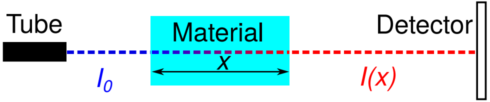
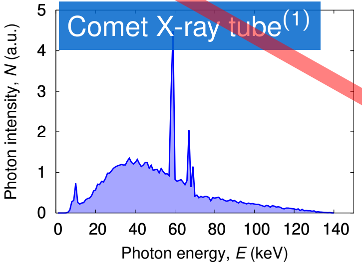


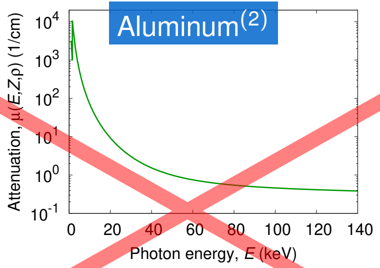
(1) Supplied by Norman Uhlmann, Fraunhofer EZRT

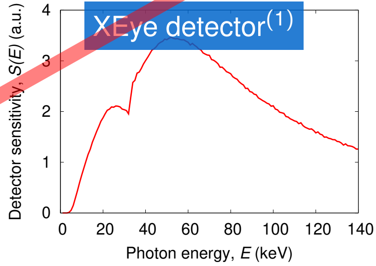
(2) XCOM supplied by NIST

Numerical approx. of $\mu_{\text{eff}}(x)$









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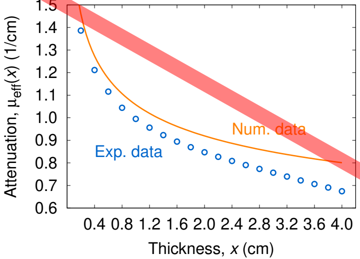
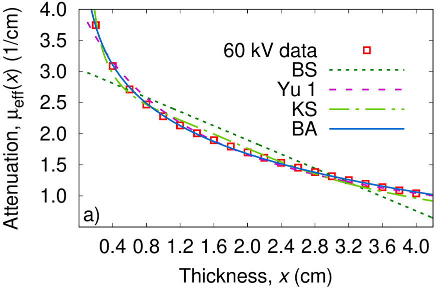


(1) Supplied by Norman Uhlmann, Fraunhofer EZRT

(2) XCOM supplied by NIST

Heuristic model functions for $\mu_{\text{eff}}(x)$



$$\mu_{\text{eff}}(x) = \mu_0 - \lambda x$$

Bjärngard & Shackford (1994)

$$\mu_{\text{eff}}(x) = \frac{\mu_0}{1+\lambda x}$$

Yu *et al.* (1997)

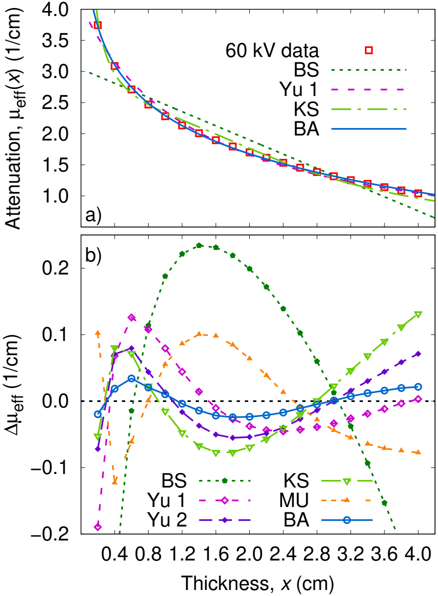
$$\mu_{\text{eff}}(x) = \mu(E_{\text{max}}) + \frac{2\mu_1}{x\sqrt{-\lambda_1^2+4\lambda_2}} \times \left[\arctan\left(\frac{\lambda_1+2\lambda_2 x}{\sqrt{-\lambda_1^2+4\lambda_2}}\right) - \arctan\left(\frac{\lambda_1}{\sqrt{-\lambda_1^2+4\lambda_2}}\right)\right]$$

Kleinschmidt (1999)

$$\boldsymbol{\mu_{\text{eff}}(x) = a + \frac{b}{x^{\alpha}}}$$

Baur *et al.* (2019)
(this work)

Heuristic model functions for $\mu_{\text{eff}}(x)$



$$\mu_{\text{eff}}(x) = \mu_0 - \lambda x$$

Bjärngard & Shackford (1994)

$$\mu_{\text{eff}}(x) = \frac{\mu_0}{1+\lambda x}$$

$$\mu_{\text{eff}}(x) = \frac{\mu_0}{(1+\lambda x)^\beta}$$

Yu *et al.* (1997)

$$\mu_{\text{eff}}(x) = \mu(E_{\text{max}}) + \frac{2\mu_1}{x\sqrt{-\lambda_1^2+4\lambda_2}} \times \left[\arctan\left(\frac{\lambda_1+2\lambda_2 x}{\sqrt{-\lambda_1^2+4\lambda_2}}\right) - \arctan\left(\frac{\lambda_1}{\sqrt{-\lambda_1^2+4\lambda_2}}\right)\right]$$

Kleinschmidt (1999)

$$\mu_{\text{eff}}(x) = -\frac{1}{x}\ln\left[A + B\exp(-x/C)\right]$$

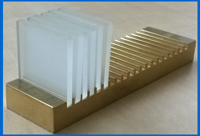
Mudde *et al.* (2008)

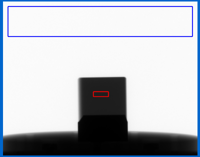
$$\boxed{\mu_{\text{eff}}(x) = a + \frac{b}{x^\alpha}}$$

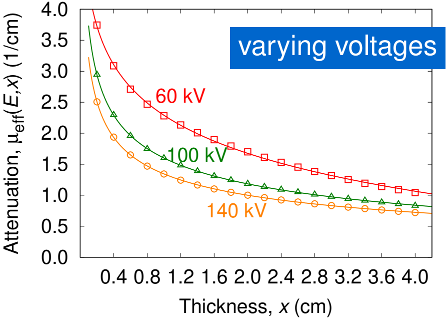
Baur *et al.* (2019)

(this work)

Universality of $\mu_{\text{eff}}(x) = a + \frac{b}{x^{\alpha}}$







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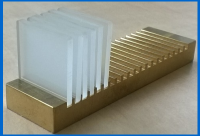

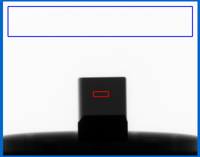

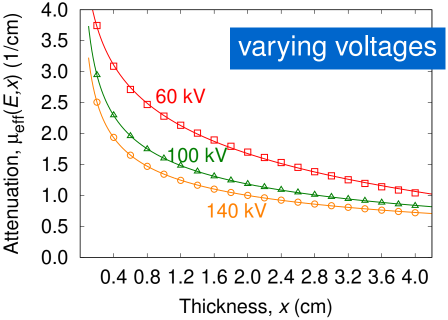

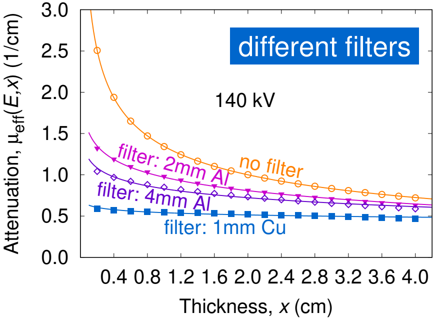

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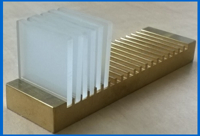

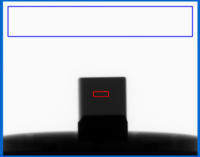

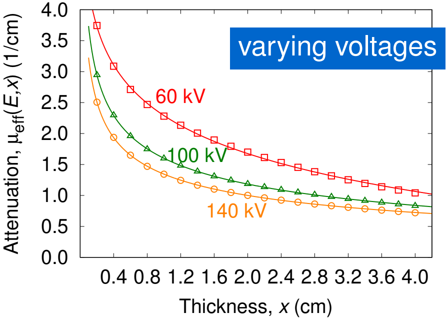

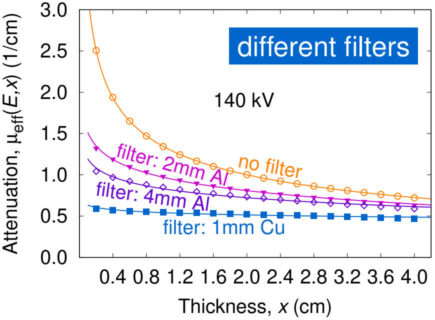

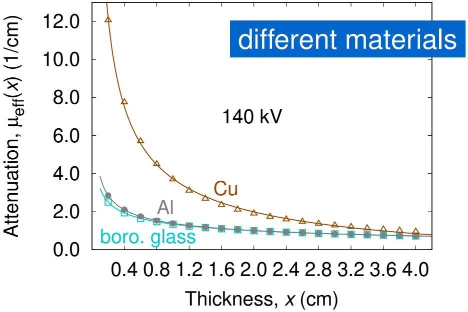

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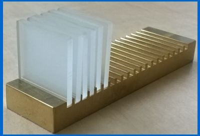
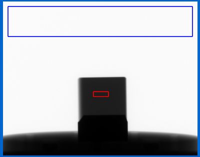
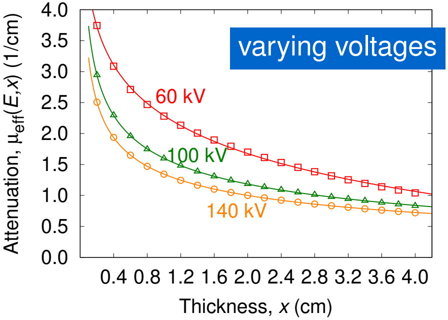
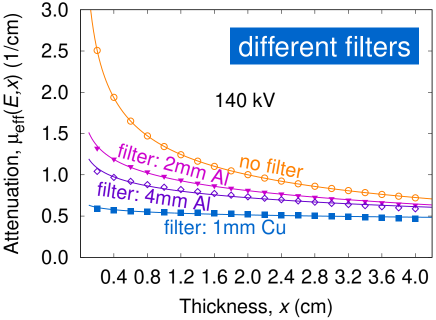
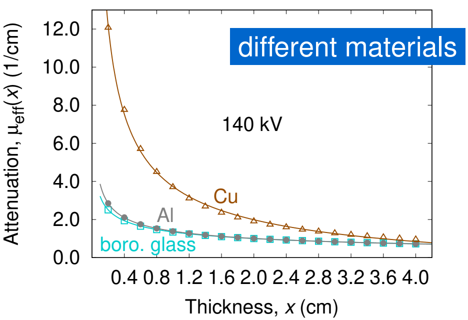
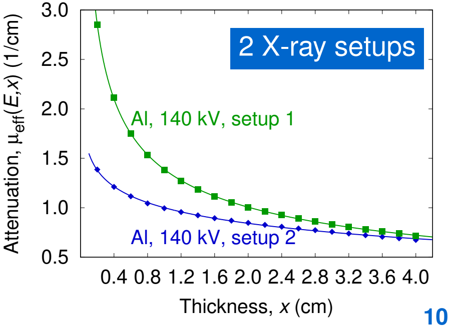












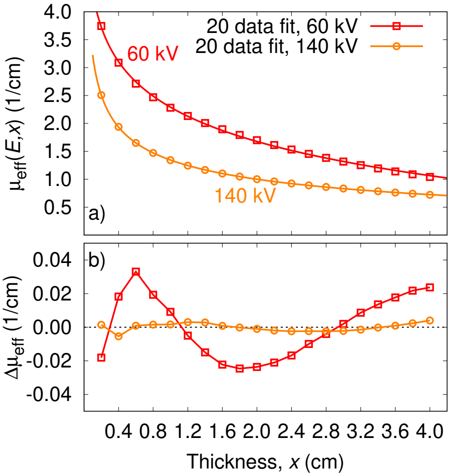
Determining the material thickness x

Generalized Beer-Lambert

$$I(x) = I_0 \exp(-\mu_{\text{eff}}(x)\, x)$$

Model function

$$\mu_{\text{eff}}(x) = a + \frac{b}{x^{\alpha}}$$



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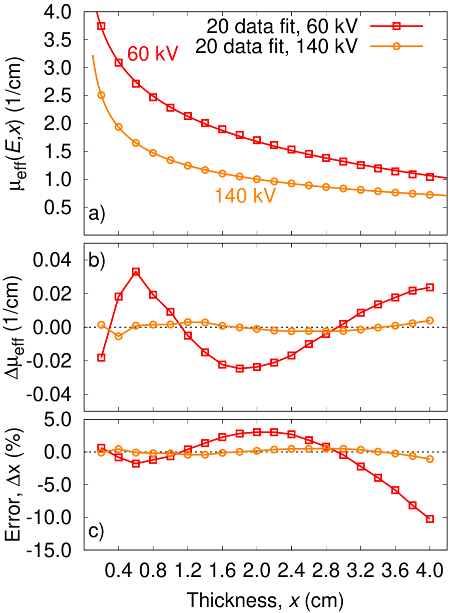
$$ax + bx^{1-\alpha} + \ln\left(\frac{I(x)}{I_0}\right) = 0$$

e.g. Newton's method or look-up table



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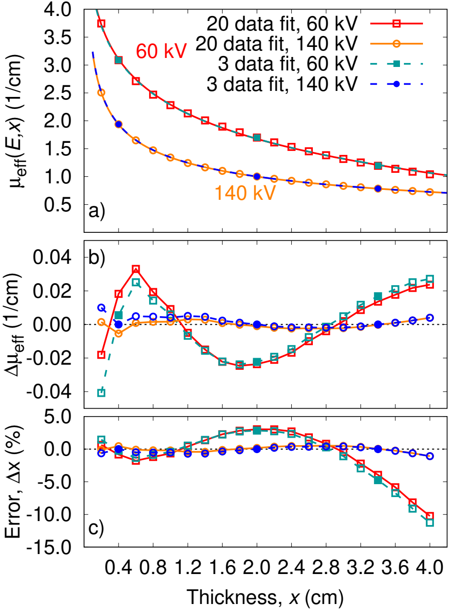
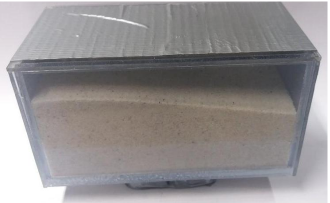
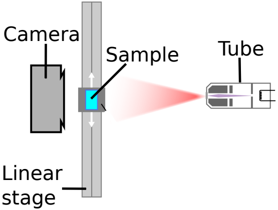
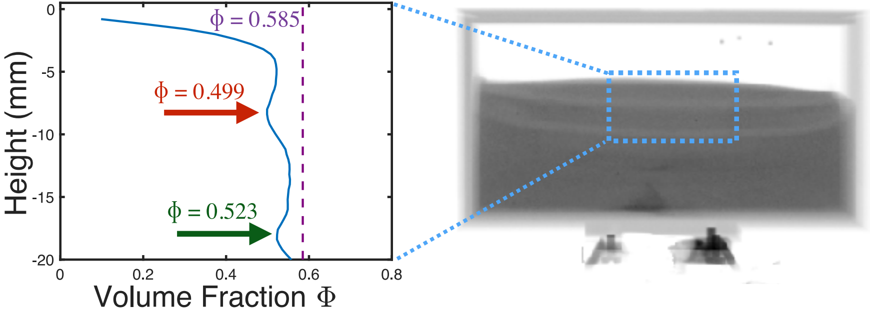


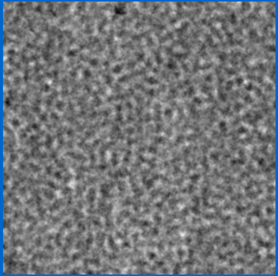
Migrating shear bands in shaken granular matter, Kollmer *et al* (2020)





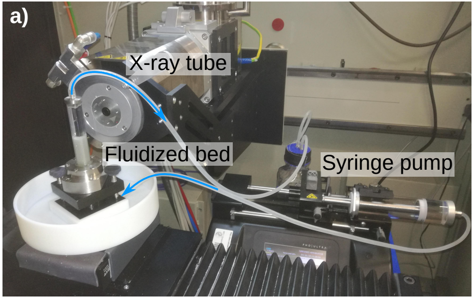


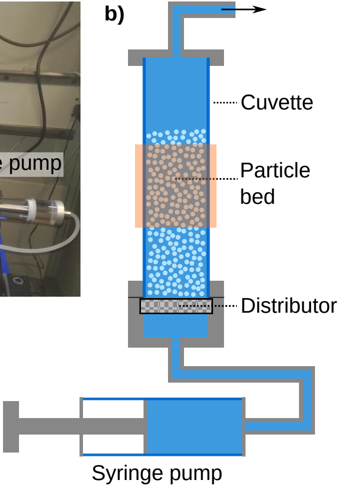
Measuring granular dynamics with
X-ray Digital Fourier Analysis (X-DFA)

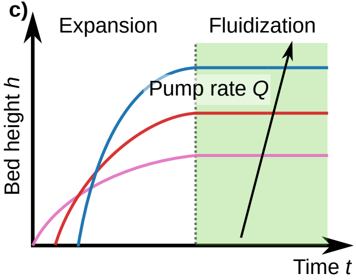


In collaboration with M. Escobedo & S. Egelhaaf, University of Düsseldorf

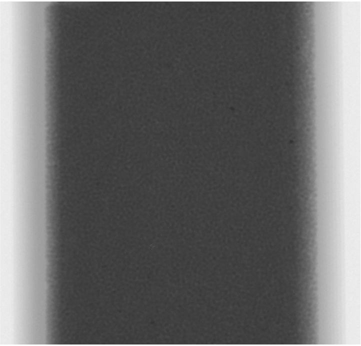
The system: A liquid fluidized bed







Radiogram



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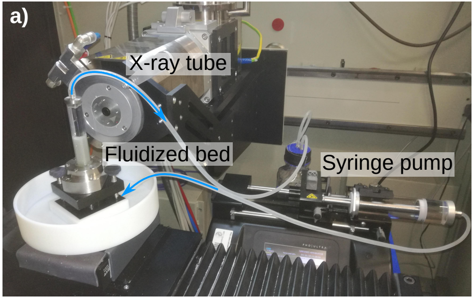
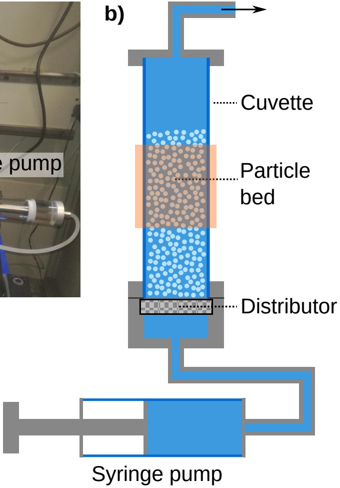
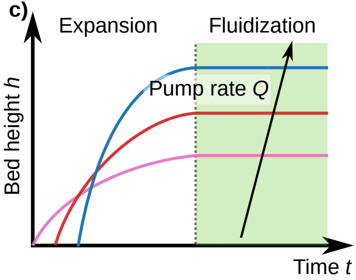
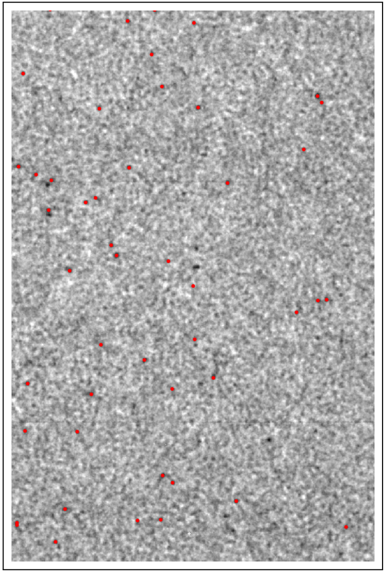






Particle tracking

Contrast: $\rho_{\text{tracer}} > \rho_{\text{bed}}$



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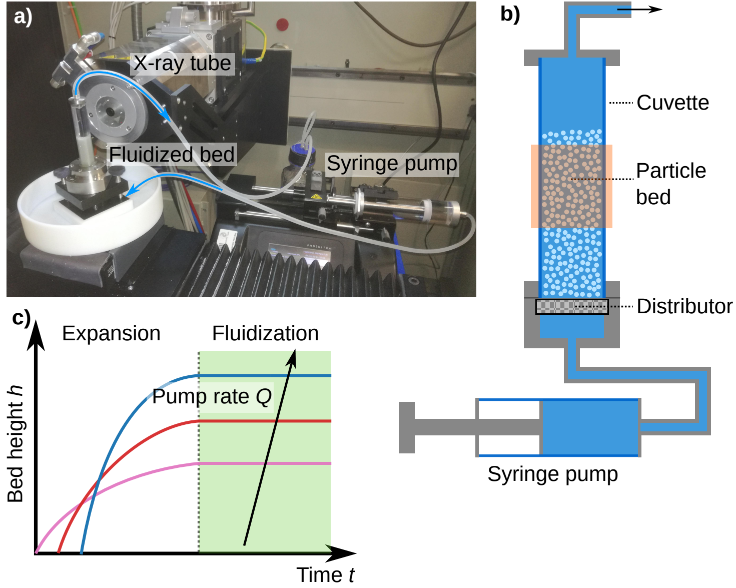

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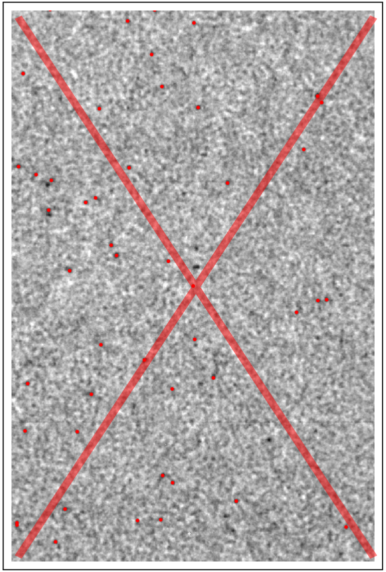

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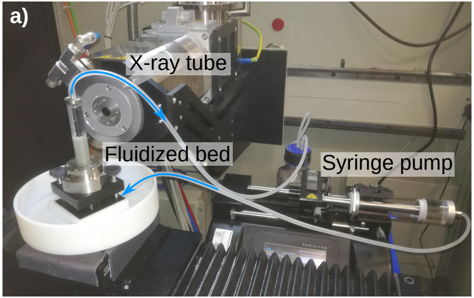
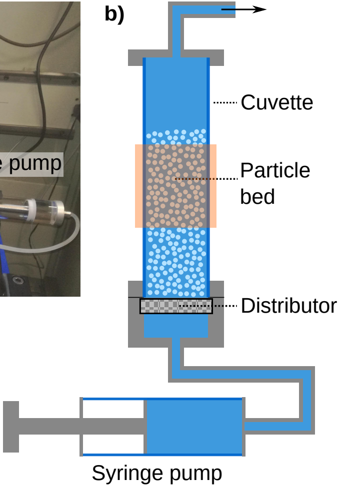
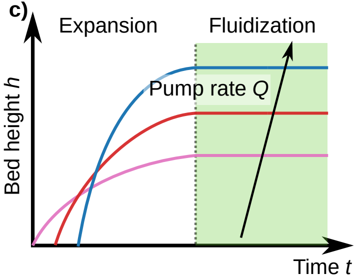
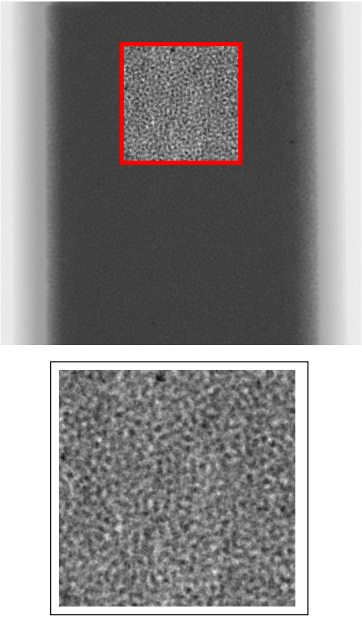






Radiogram



Differential Dynamic Microscopy (DDM)

	Up to now	**This work**
System	Dispersion, gels	Fluidized bed
Particles	Colloids < 1 µm	Granulates $(150 - 180)$ µm
Volume fraction	$\Phi \leq 0.33$	$0.45 < \Phi < 0.56$
imaging	Light microscopy	X-ray radiography
Dynamics	Brownian motion, caging, glassy, collective motion	

Giavazzi *et al*, PRE **80**, 031403 (2009)

Extending Differential Dynamic Microscopy (DDM) to X-ray imaging

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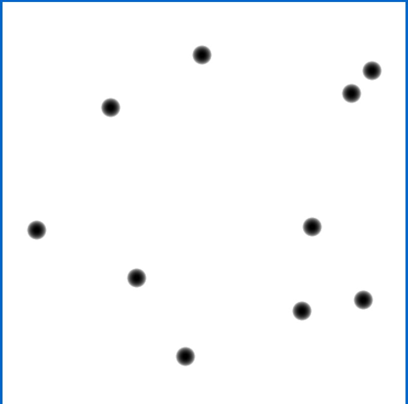
Digital Fourier Analysis of X-Ray radiograms (X-DFA)

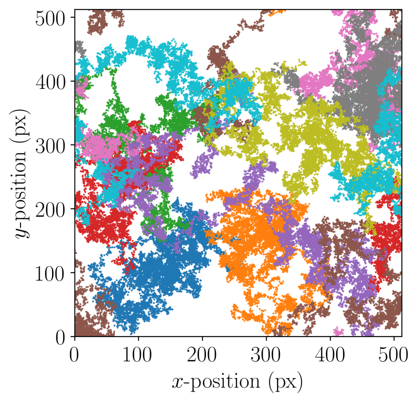
Giavazzi *et al*, PRE **80**, 031403 (2009)

Introduction to
X-ray Digital Fourier Analysis (X-DFA)

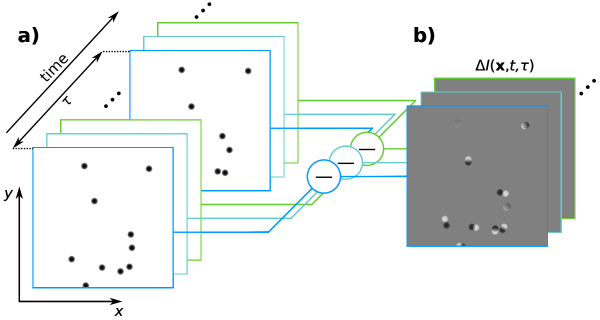
Synthetic radiograms



Particle trajectory



The image structure function $D(\mathbf{q}, \tau)$



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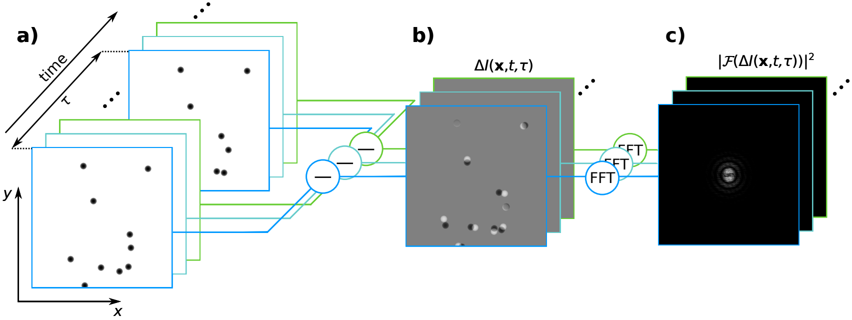

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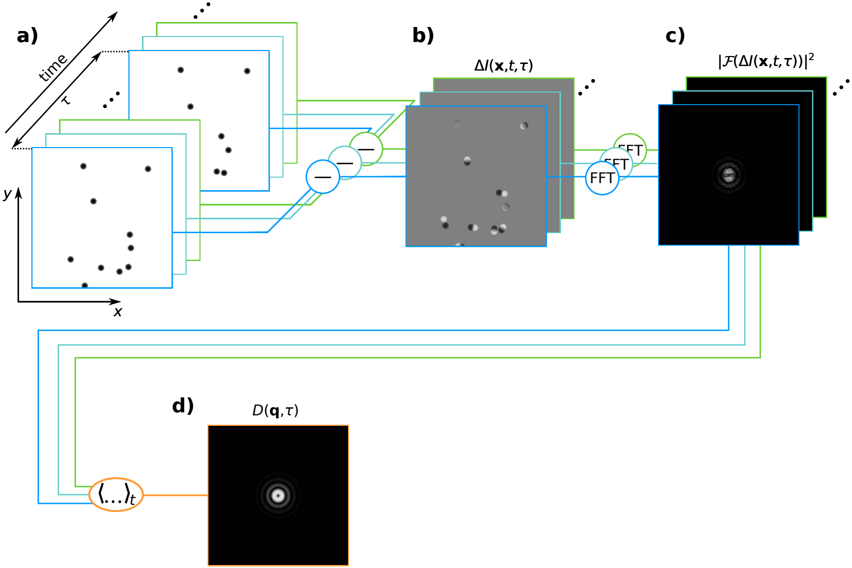

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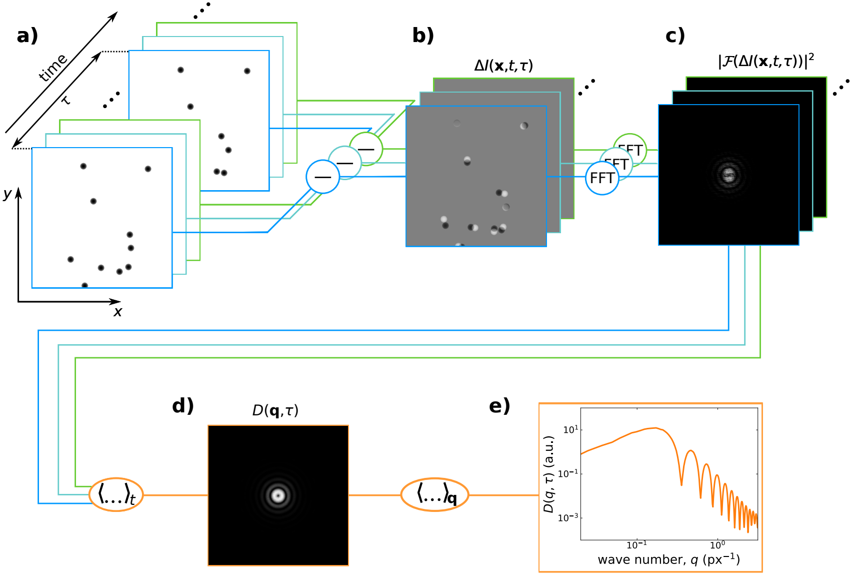

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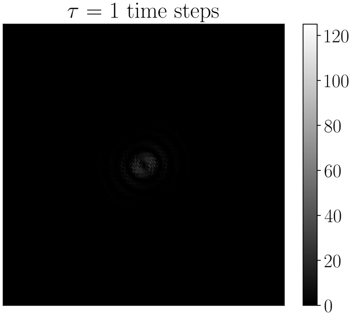
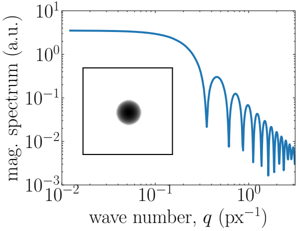
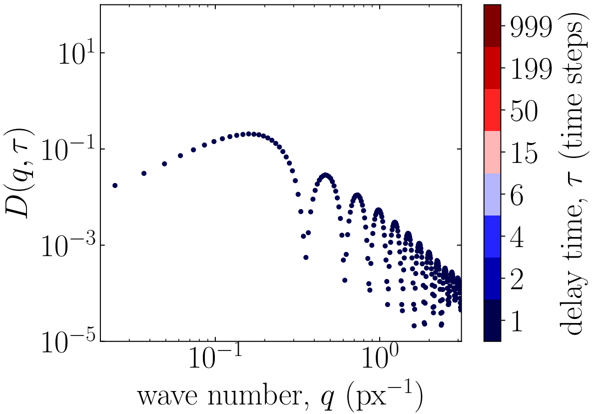




Time averaging: $D(\mathbf{q}, \tau) = \langle |\mathscr{F}(\Delta I)|^2 \rangle_t$

Azimuthal averaging: $D(\mathbf{q}, \tau) \rightarrow D(q, \tau)$ ...



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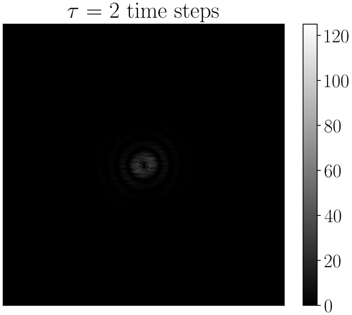

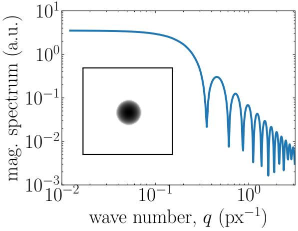

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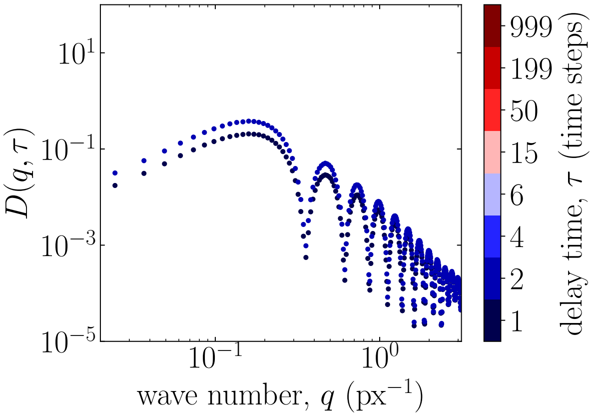

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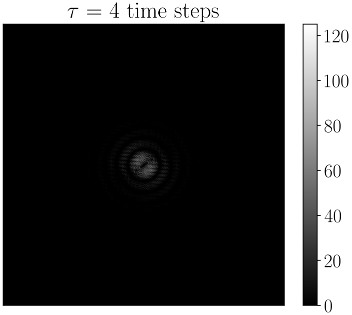

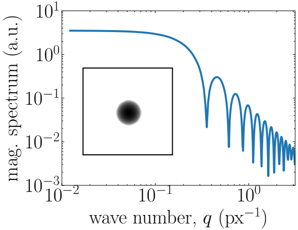

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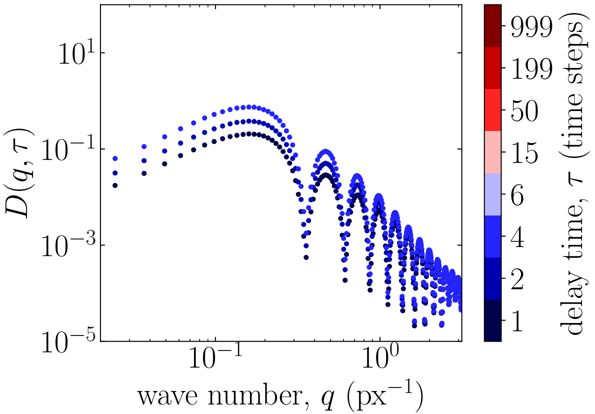

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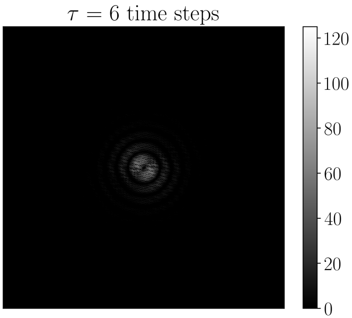

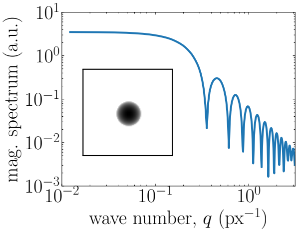

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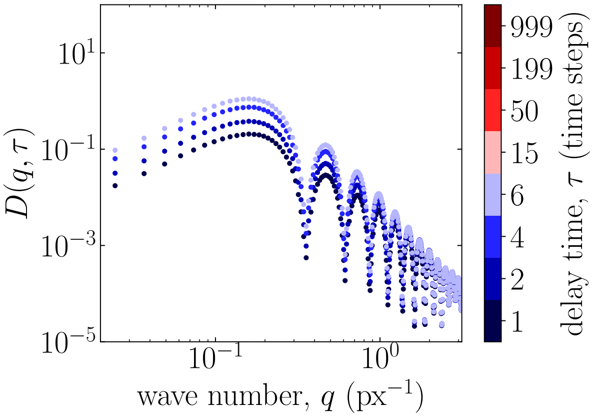

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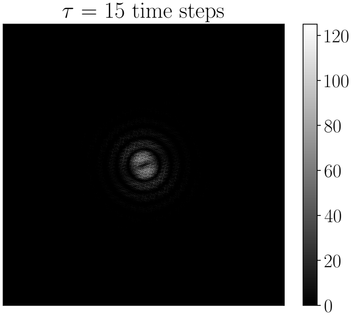

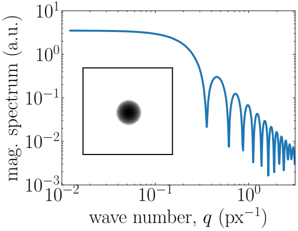

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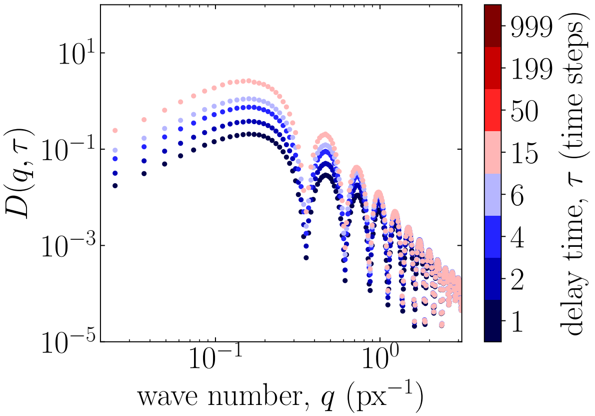
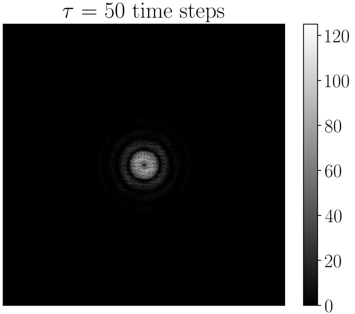
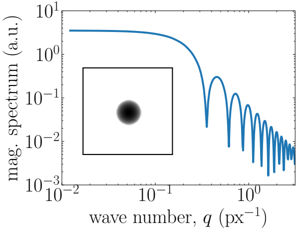


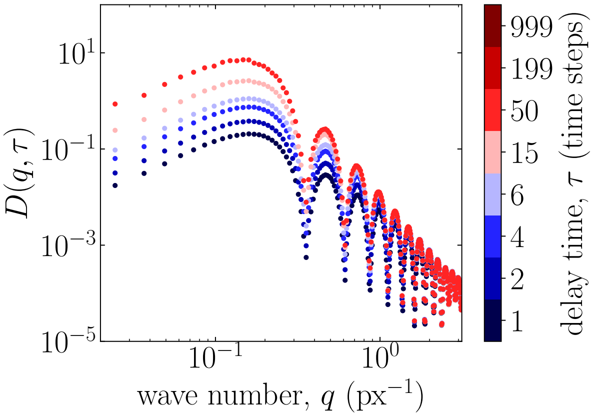
The image structure function $D(q, \tau)$



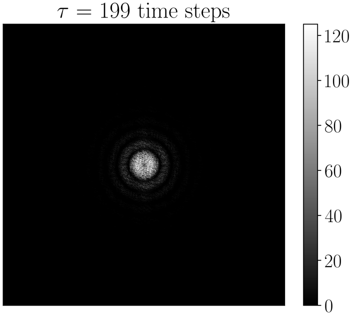


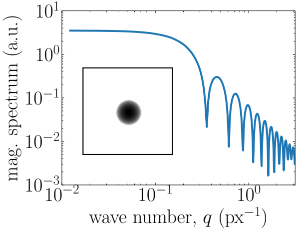
Time averaging: $D(\mathbf{q}, \tau) = \langle |\mathscr{F}(\Delta I)|^2 \rangle_t$

Azimuthal averaging: $D(\mathbf{q}, \tau) \rightarrow D(q, \tau)$ ...



The image structure function $D(q, \tau)$





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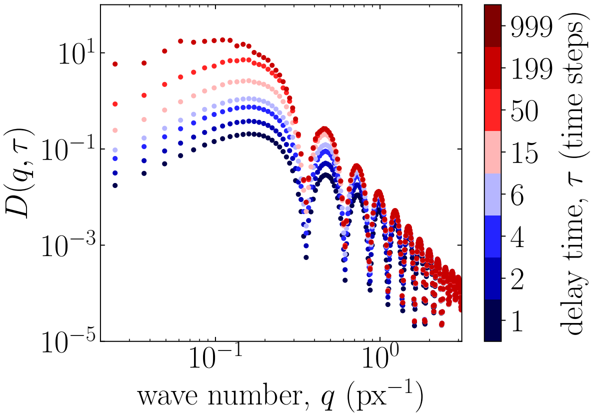

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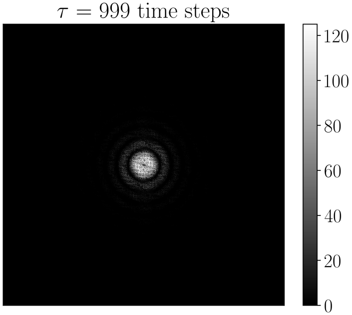

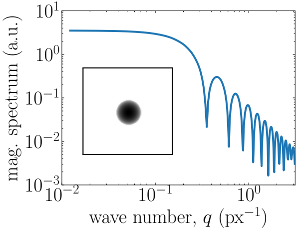

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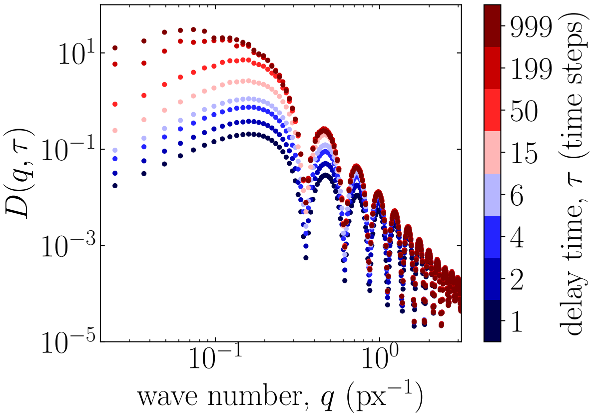

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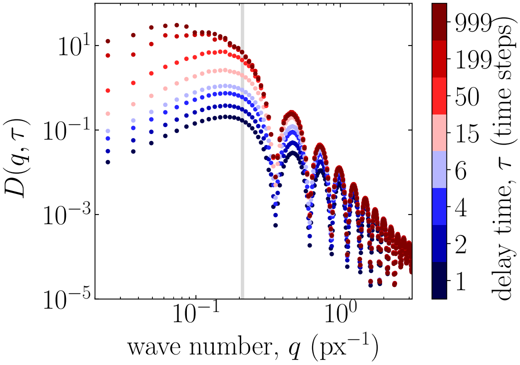
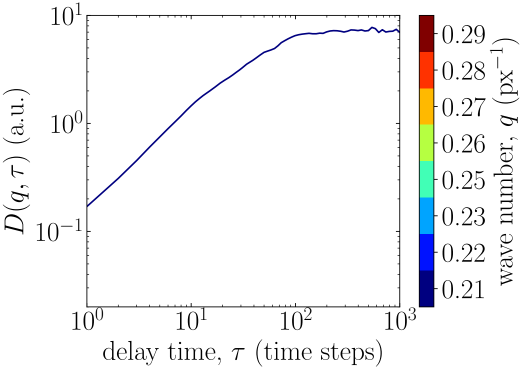
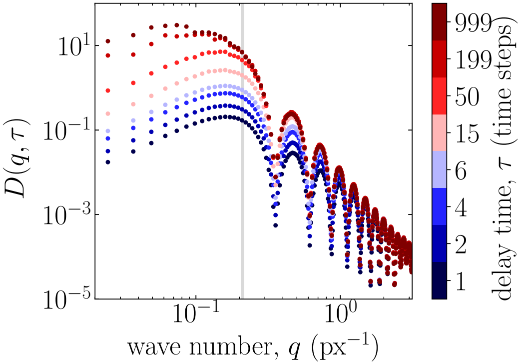
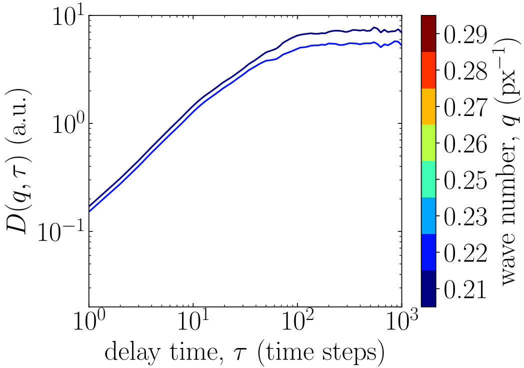




The image structure function $D(q, \tau)$





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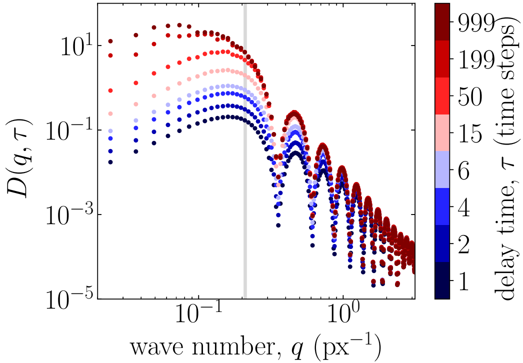

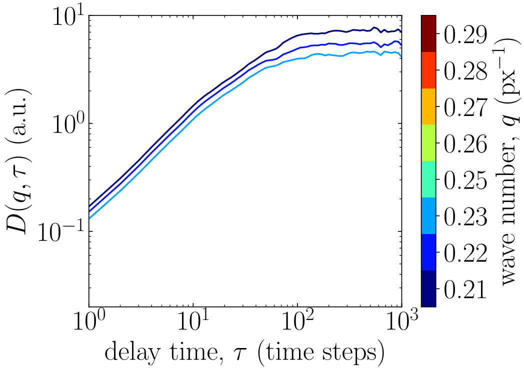

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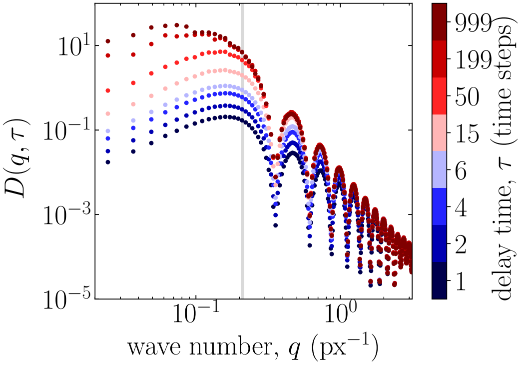
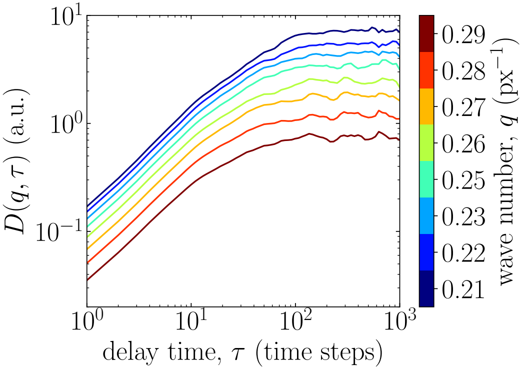
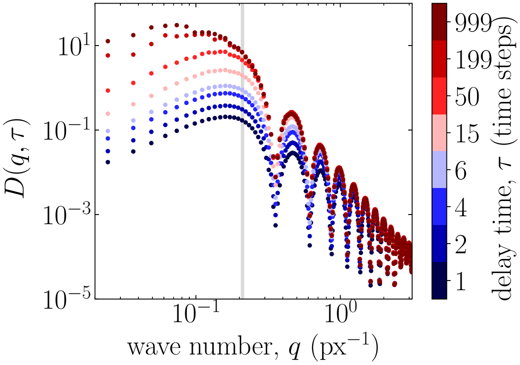
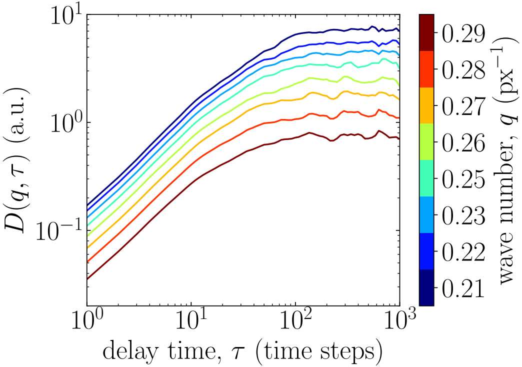




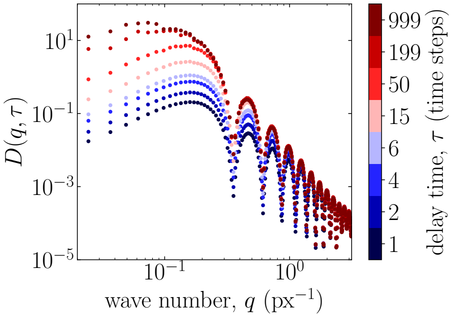
$$
\begin{aligned}
D(q,\tau) &= \left\langle |I(q, t+\tau) - I(q,t)|^2 \right\rangle_t \\
&= A(q)\left[1 - \frac{\langle I^*(q,t) I(q,t+\tau)\rangle_t}{\langle |I(q,t)|^2\rangle_t}\right] + B(q)
\end{aligned}
$$

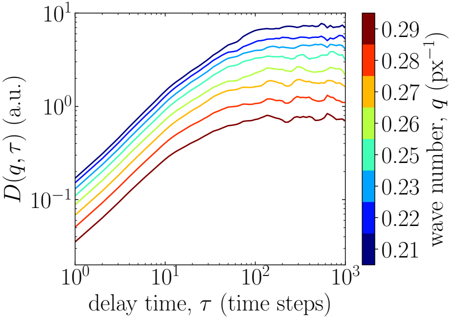
The image structure function $D(q, \tau)$





$$
\begin{aligned}
D(q,\tau) &= \left\langle |I(q,t+\tau) - I(q,t)|^2 \right\rangle_t \\
&= A(q)\left[1 - \underbrace{\frac{\left\langle I^*(q,t)I(q,t+\tau)\right\rangle_t}{\left\langle |I(q,t)|^2\right\rangle_t}}_{\text{Image correlation function}}\right] + B(q)
\end{aligned}
$$





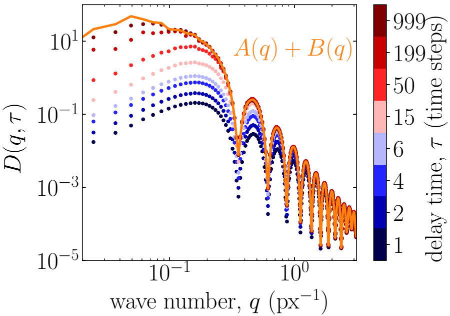
$$D(q,\tau) = \left\langle |I(q,t+\tau) - I(q,t)|^2 \right\rangle_t$$

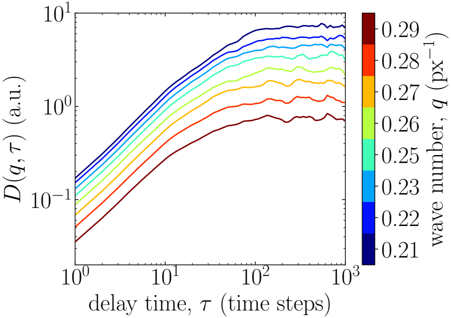
$$= A(q)\left[1 - \underbrace{\frac{\left\langle I^*(q,t)I(q,t+\tau)\right\rangle_t}{\left\langle |I(q,t)|^2\right\rangle_t}}_{\text{Image correlation function}}\right] + B(q)$$

Linear space invariant imaging

$$f(q,\tau) = \frac{\langle \rho^*(q,t)\rho(q,t+\tau)\rangle_t}{\langle |\rho(q,t)|^2\rangle_t}$$

Intermediate scattering function





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- $D(q,\tau \to 0) = B(q) = 0$
- $D(q,\tau \to \infty) = A(q) + B(q)$

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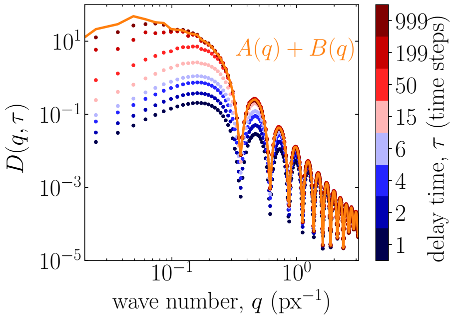

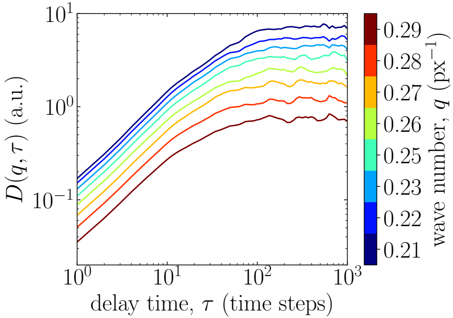

$$D(q,\tau) = \left\langle |I(q,t+\tau) - I(q,t)|^2 \right\rangle_t$$

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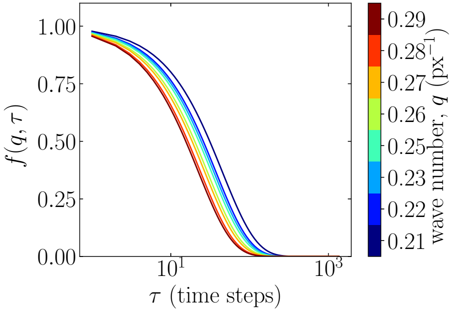
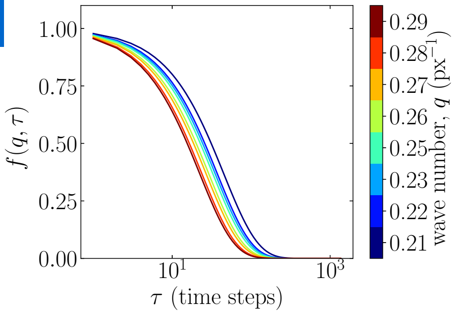


- $D(q,\tau \to 0) = B(q) = 0$
- $D(q,\tau \to \infty) = A(q) + B(q)$

Intermediate scattering function $f(q, \tau)$

Brownian motion:
$f(q, \tau) = \exp(-q^2 \tau / \tau_D)$



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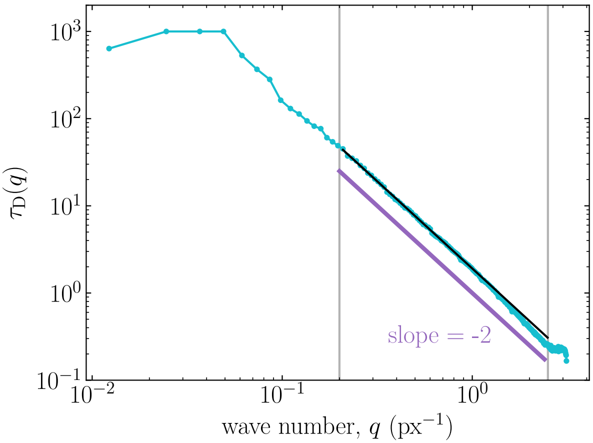
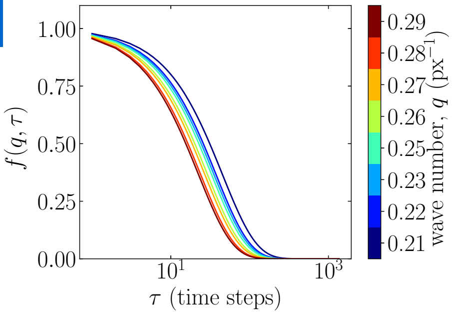
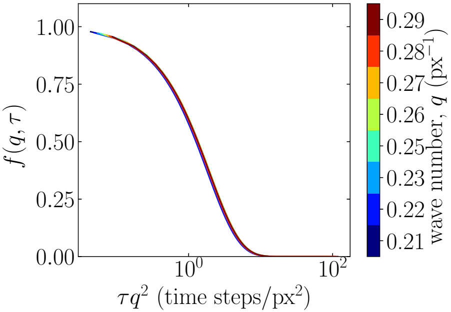
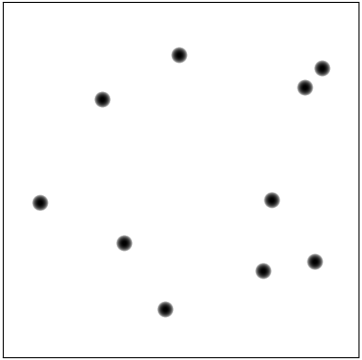




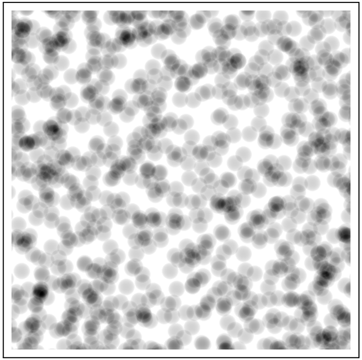


Accuracy of X-DFA: Varying the number of particles

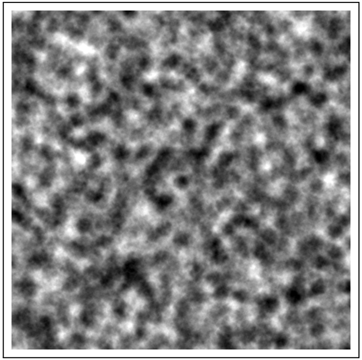
10 particles



1000 particles



100 000 particles



Deviation from the simulation input:

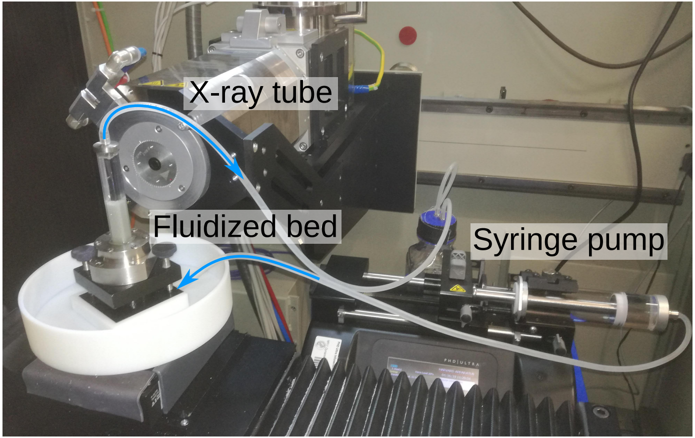
6%

2%

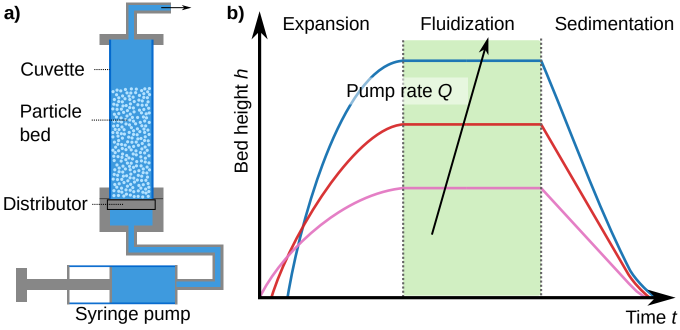
2%

PIV off by ≈ 650%

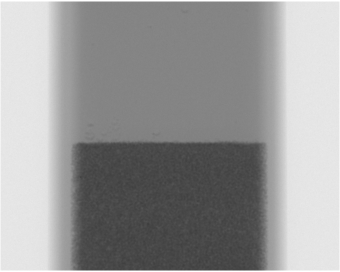
Experimental validation of X-DFA:
A suspension of sedimenting particles

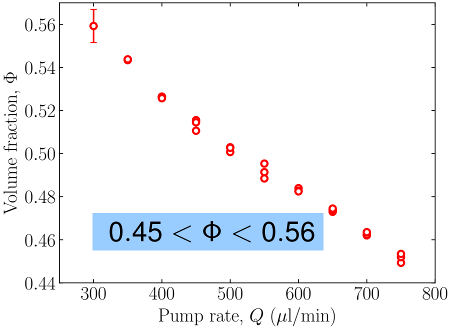


Experimental validation of X-DFA: A suspension of sedimenting particles

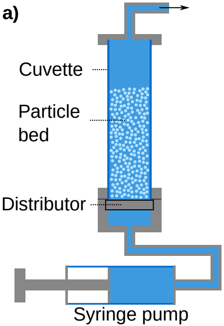


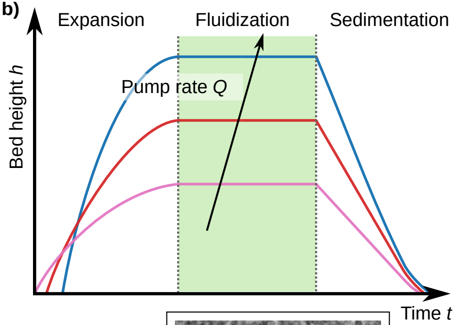
X-ray radiography



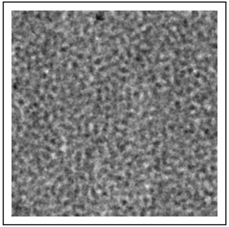


Experimental validation of X-DFA: A suspension of sedimenting particles





No reliable reference velocity!



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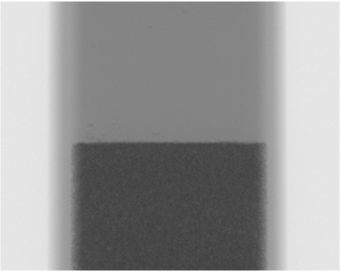
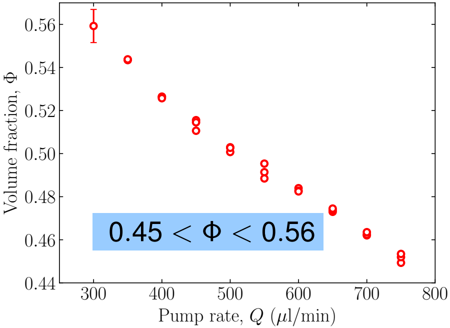
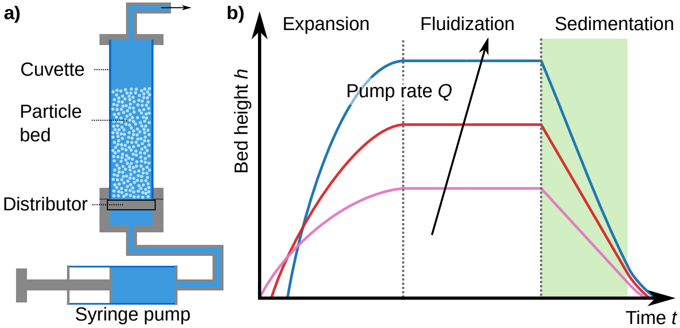




Experimental validation of X-DFA: A suspension of sedimenting particles



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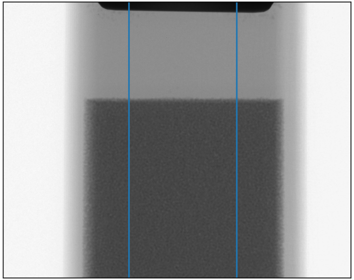
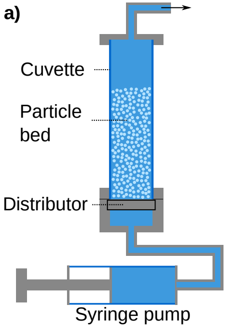
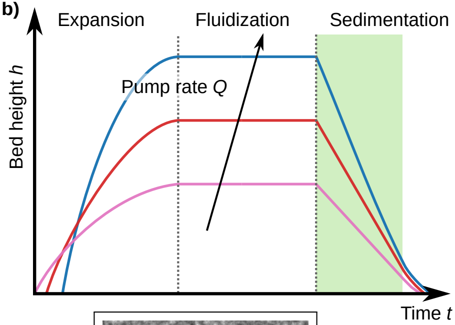
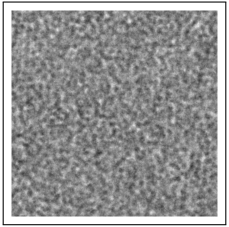


Experimental validation of X-DFA: A suspension of sedimenting particles

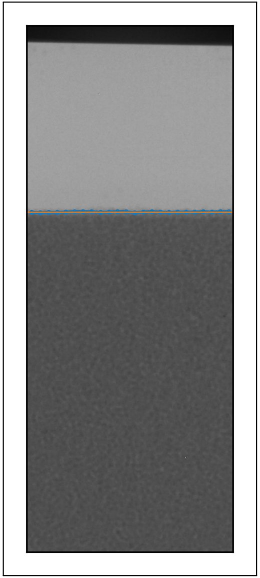




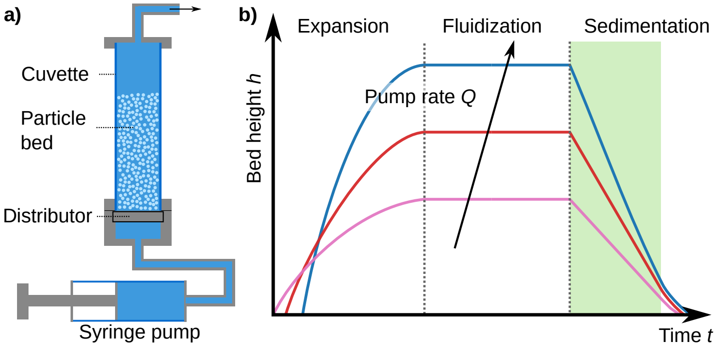


Comparison of $\langle v \rangle_{\mathrm{xdfa}}$ and $\langle v \rangle_{\mathrm{front}}$

X-ray radiography



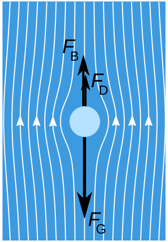
Liquid fluidized bed: Richardson-Zaki law



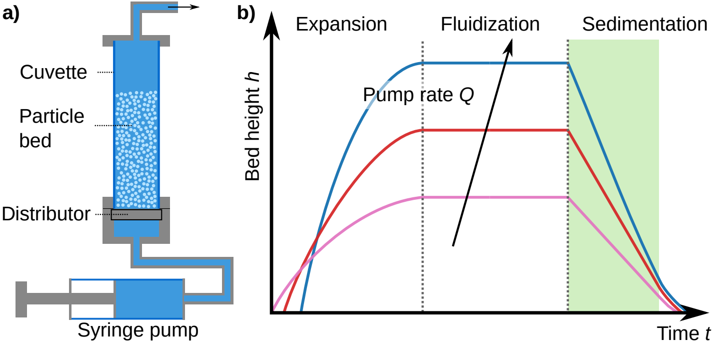
$$\frac{\langle v \rangle_{\text{fluid}}}{v_{\text{Stokes}}} = (1 - \Phi)^n$$

Gravitation Buoyancy Drag

$$F_G = F_B + F_D$$



Liquid fluidized bed: Richardson-Zaki law



Gravitation Buoyancy Drag

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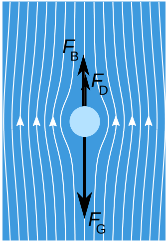
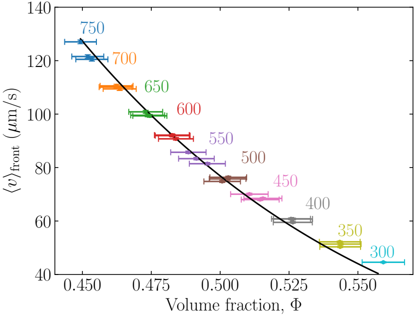
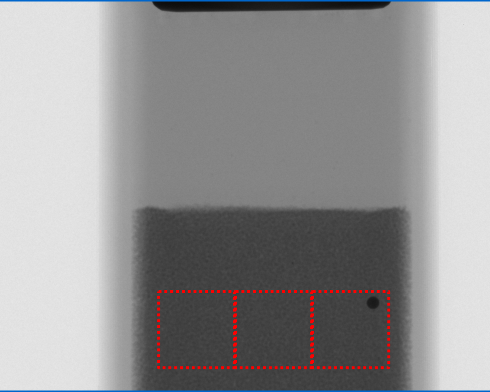
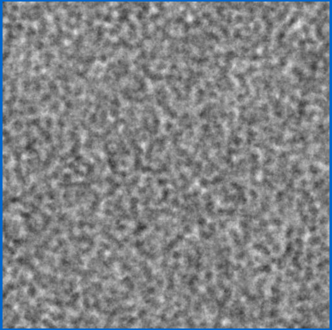


$$\frac{\langle v \rangle_{\text{front}}}{v_{\text{Stokes}}} = (1 - \Phi)^n$$

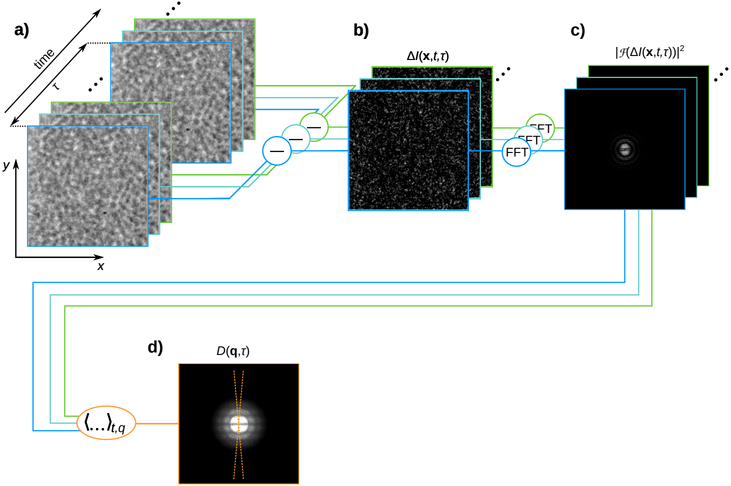


X-ray Digital Fourier Analysis of a suspension of sedimenting particles



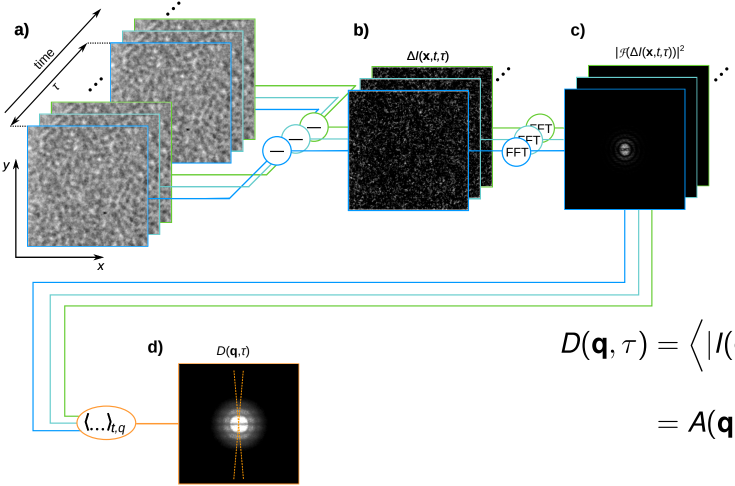


The image structure function $D(\mathbf{q}, \tau)$



In collaboration with Manuel Escobedo, University of Düsseldorf

The image structure function $D(\mathbf{q}, \tau)$



$$D(\mathbf{q}, \tau) = \left\langle |I(\mathbf{q}, t+\tau) - I(\mathbf{q}, t)|^2 \right\rangle_t$$

$$= A(\mathbf{q}) \left[1 - \frac{\left\langle I^*(\mathbf{q}, t) I(\mathbf{q}, t+\tau) \right\rangle_t}{\left\langle |I(\mathbf{q}, t)|^2 \right\rangle_t} \right] + B(\mathbf{q})$$

- $D(\mathbf{q}, \tau \to 0) = B(\mathbf{q})$
- $D(\mathbf{q}, \tau \to \infty) = A(\mathbf{q}) + B(\mathbf{q})$

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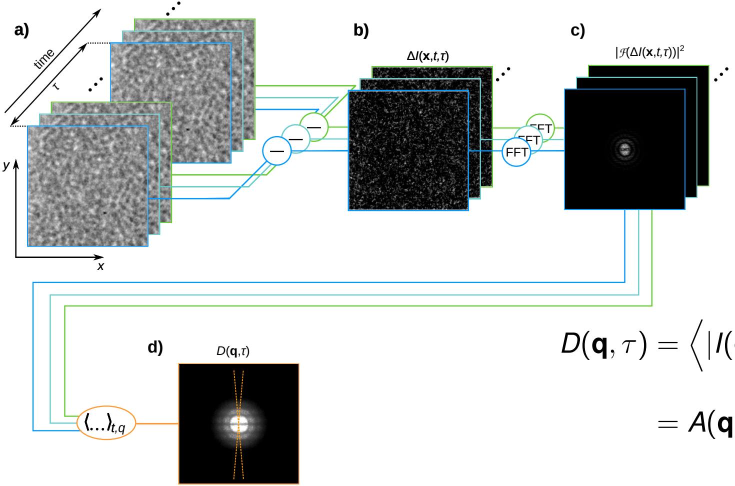
The image structure function $D(\mathbf{q}, \tau)$



Linear space invariant imaging

$$f(\mathbf{q}, \tau) = \frac{\langle \rho^*(\mathbf{q}, t)\rho(\mathbf{q}, t+\tau)\rangle_t}{\langle |\rho(\mathbf{q}, t)|^2\rangle_t}$$

Intermediate scattering function

$$D(\mathbf{q}, \tau) = \left\langle |I(\mathbf{q}, t+\tau) - I(\mathbf{q}, t)|^2 \right\rangle_t$$

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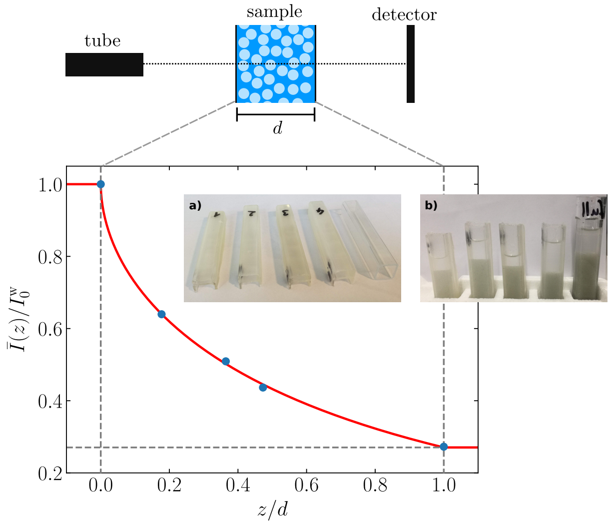
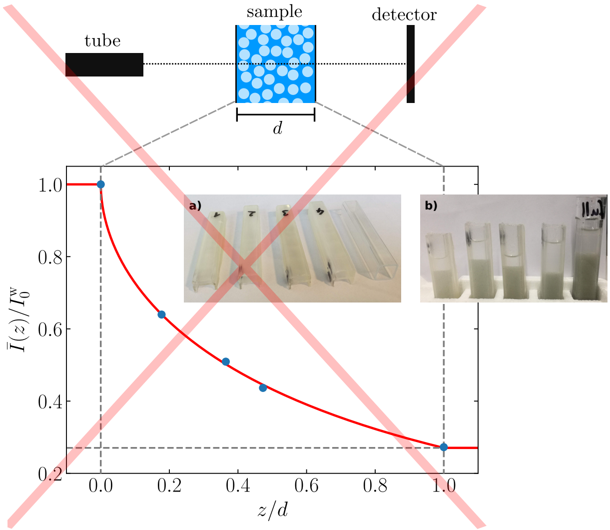
In collaboration with Manuel Escobedo, University of Düsseldorf

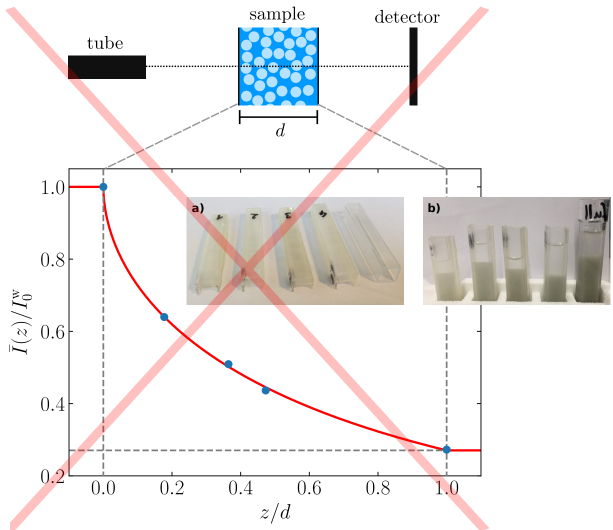
X-ray imaging – Linear space invariant?

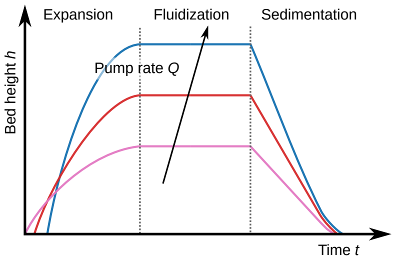


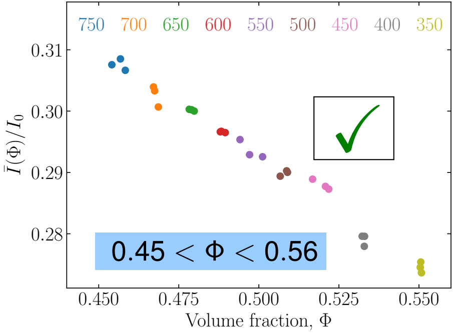
X-ray imaging – Linear space invariant?



X-ray imaging – Linear space invariant?



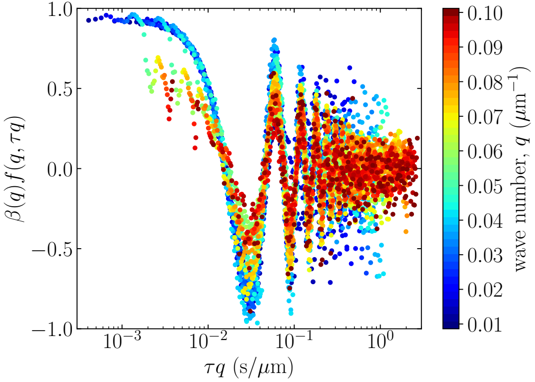


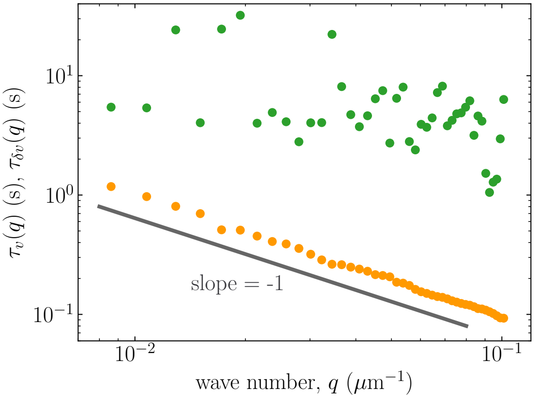


X-DFA for a suspension of sedimenting particles

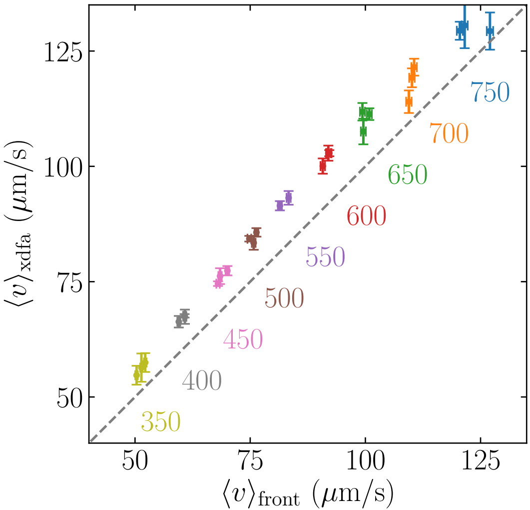
$$f(q,\tau) = \cos(q\langle v_s\rangle\tau)\exp\left(-\frac{1}{2}q^2\delta v^2\tau^2\right)$$

$$\langle v_s\rangle = \langle\Delta r\rangle/\tau_\nu, \langle\delta v\rangle = \langle\delta r\rangle/\tau_{\delta\nu}$$



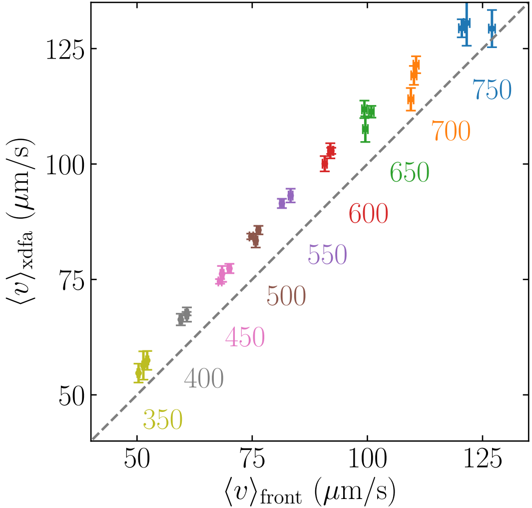


Front tracking vs. X-DFA

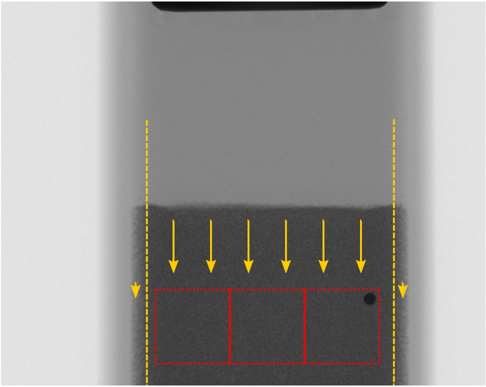


$\langle v \rangle_{\text{xdfa}} > \langle v \rangle_{\text{front}}$ by 9.4%

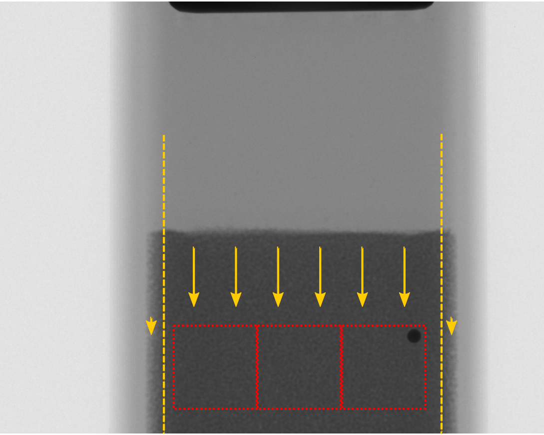
Front tracking vs. X-DFA



$\langle v \rangle_{\mathrm{xdfa}} > \langle v \rangle_{\mathrm{front}}$ by 9.4%

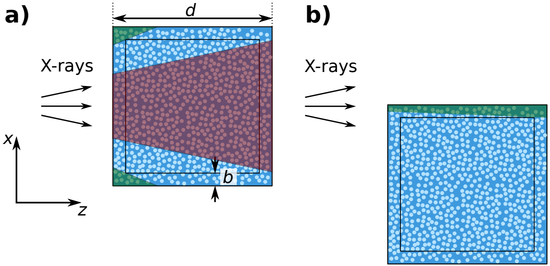


Estimate width of boundary layer



$\langle v \rangle_{\mathrm{xdfa}} > \langle v \rangle_{\mathrm{front}}$ by 9.4%

$\langle v \rangle_{\mathrm{xdfa}}$ takes two layers into account
$\langle v \rangle_{\mathrm{front}}$ takes four layers into account

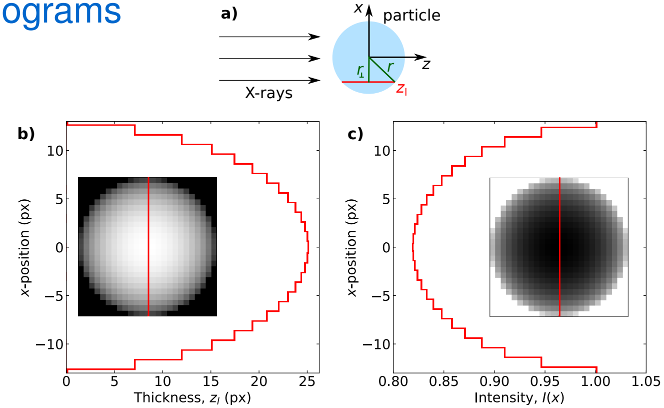


Estimation:
Boundary velocity = 0
Else = const.
$\rightarrow b \approx 3$ particle diameters


Thank you for your attention!
3000 µl/min
3500 µl/min
4000 µl/min

Backup slides

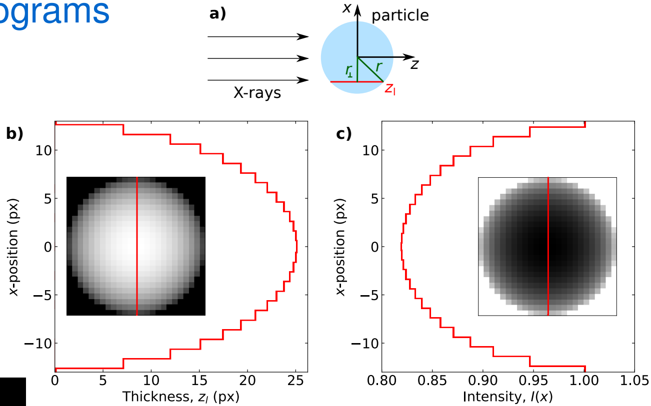
Synthetic radiograms

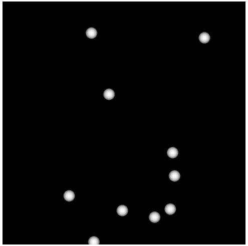


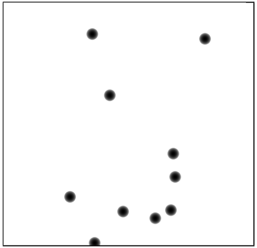
Beer-Lambert

$$I(z_l) = I_0 \exp(-\mu z)$$

Synthetic radiograms







Beer-Lambert

$$I(z_l) = I_0 \exp(-\mu z)$$

Linear space invariant imaging

Image correlation function

$$g(\mathbf{q}, \tau) = \frac{\langle I^*(\mathbf{q}, t) I(\mathbf{q}, t + \tau) \rangle_t}{\langle |I(\mathbf{q}, t)|^2 \rangle_t}$$

Linear space invariant imaging

Image correlation function

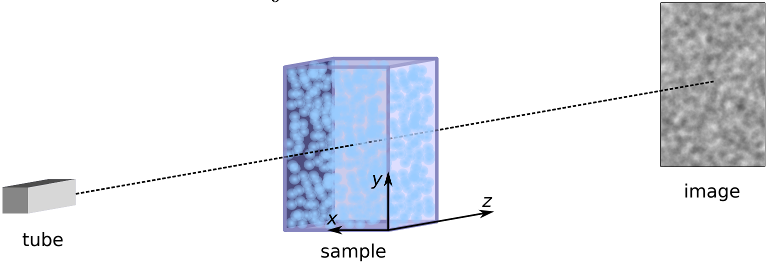
$$g(\mathbf{q},\tau) = \frac{\langle I^*(\mathbf{q},t)I(\mathbf{q},t+\tau)\rangle_t}{\langle |I(\mathbf{q},t)|^2\rangle_t}$$

Intermediate scattering function

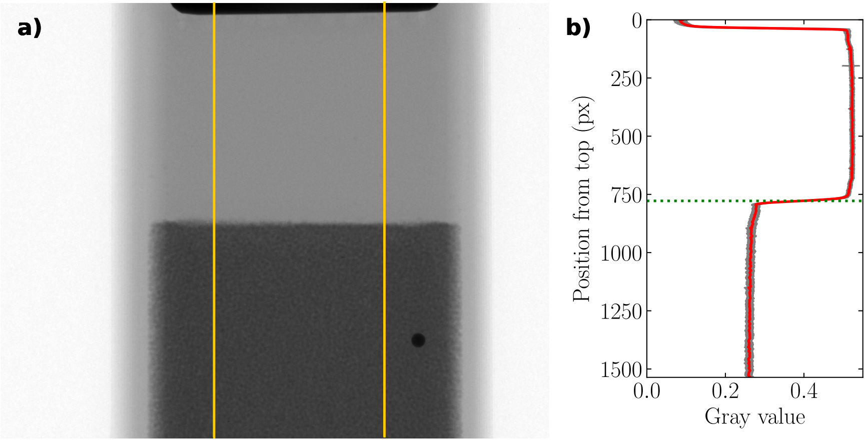
$$f(\mathbf{q},\tau) = \frac{\langle \rho^*(\mathbf{q},t)\rho(\mathbf{q},t+\tau)\rangle_t}{\langle |\rho(\mathbf{q},t)|^2\rangle_t}$$

Linear space-invariant imaging:

$$I(\mathbf{r},t) = I_0 + \int \mathrm{d}\mathbf{r}'\,\mathrm{d}z'\,T(\mathbf{r}-\mathbf{r}',-z')c(\mathbf{r}',z',t)$$



Tracking of particle front



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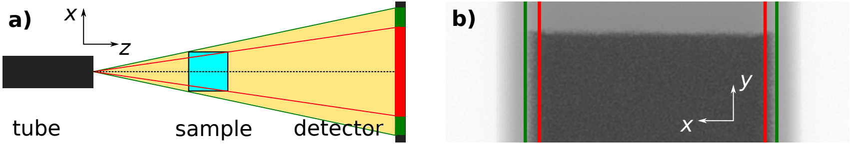

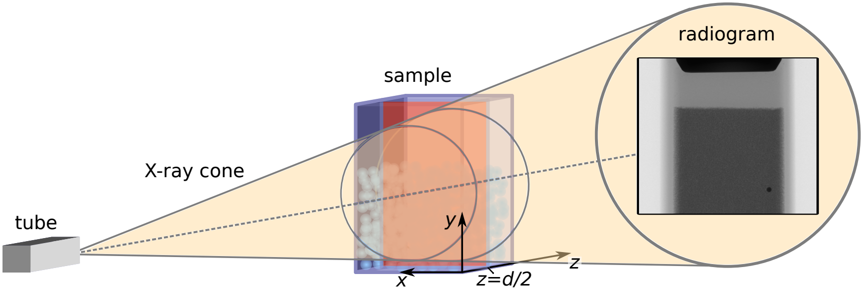

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