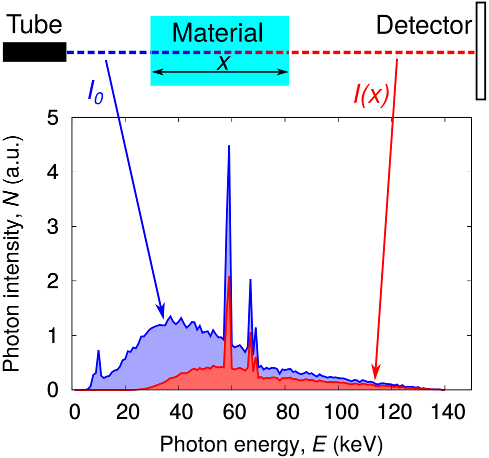
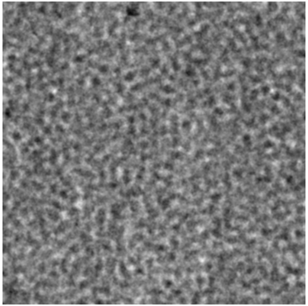
FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

Institute for
Multiscale Simulation
MSS

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





PhD defense
Manuel Baur

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

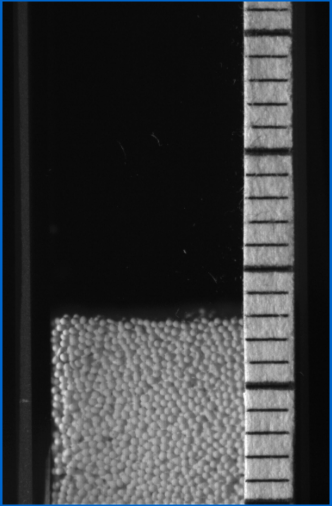
Granular flows

rough structure - replace text by images:

1. Motivate physical system of granular flow (nice challenge to study)
2. Motivate technique of radiography

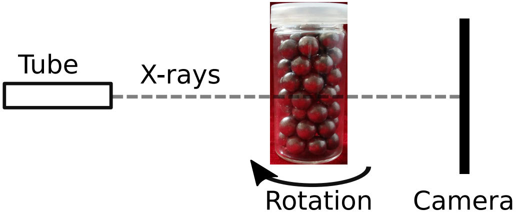
- Granular flows - fluidized bed reactors
- optically opaque
- X-ray reveal the inside
- Tomography: full 3D information - but slow (no dynamics)
- Radiography: single projections - knowledge on imaging physics
- Here two techniques to quantify: densities & dynamics

Particulate flows are **opaque**

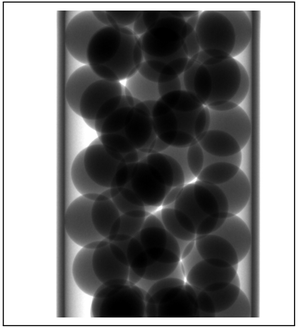


Master thesis Welm Pätzold

X-ray radiography



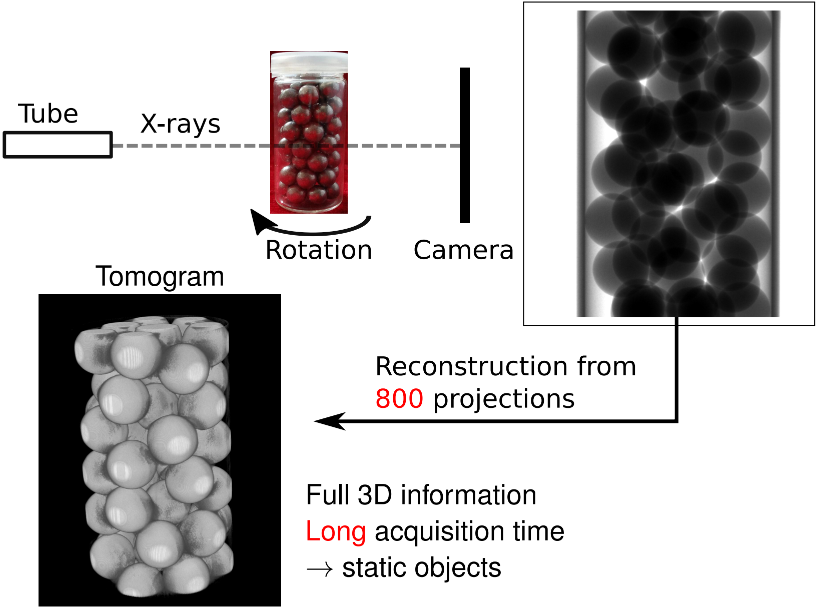
Radiogram



2D projections of 3D object

Short acquisition time

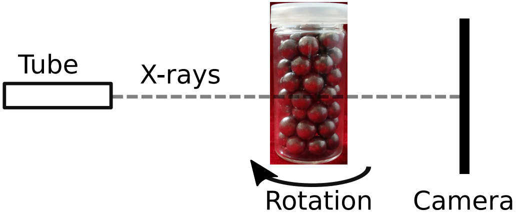
X-ray radiography



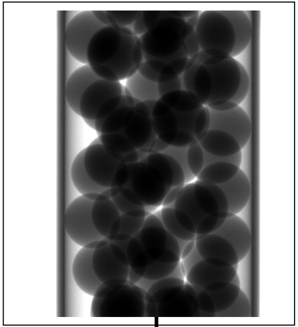
2D projections of 3D object
Short acquisition time

Full 3D information
Long acquisition time
→ static objects

X-ray radiography

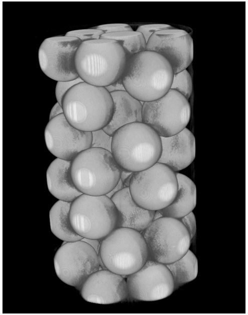


Radiogram



2D projections of 3D object
Short acquisition time

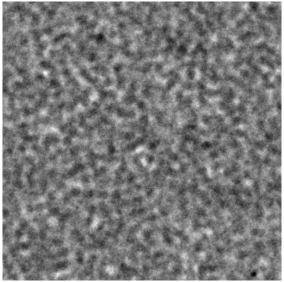
Tomogram



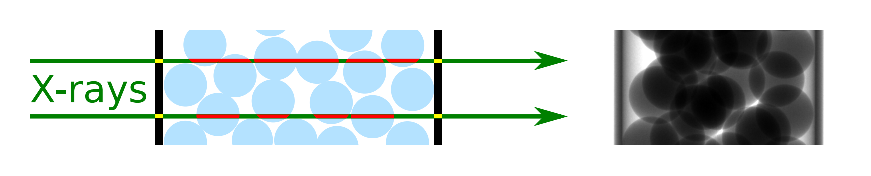
Reconstruction from
800 projections

Full 3D information
Long acquisition time
$\rightarrow$ static objects

Dynamic system



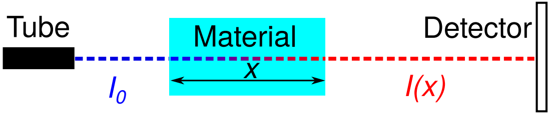
Measuring the volume fraction of **dynamic** granular systems



Correction of beam hardening in X-ray radiograms

In collaboration with Norman Uhlmann, Fraunhofer EZRT

Attenuation of X-rays

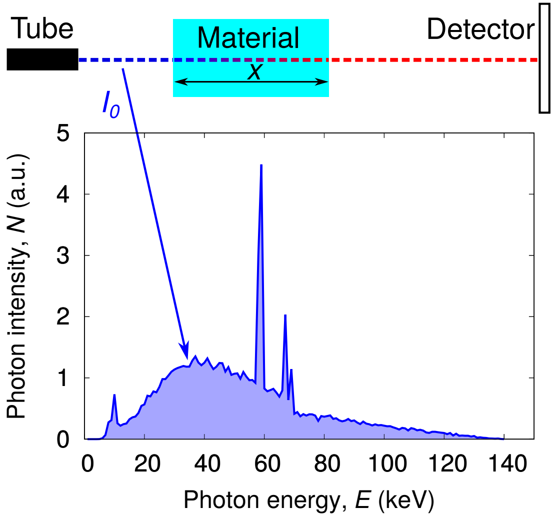


Beer-Lambert's law

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

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

Attenuation of X-rays

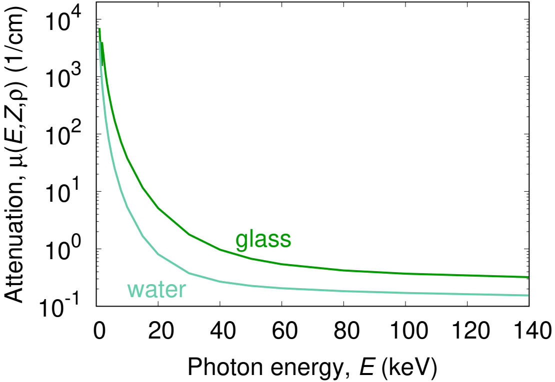


Beer-Lambert's law

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

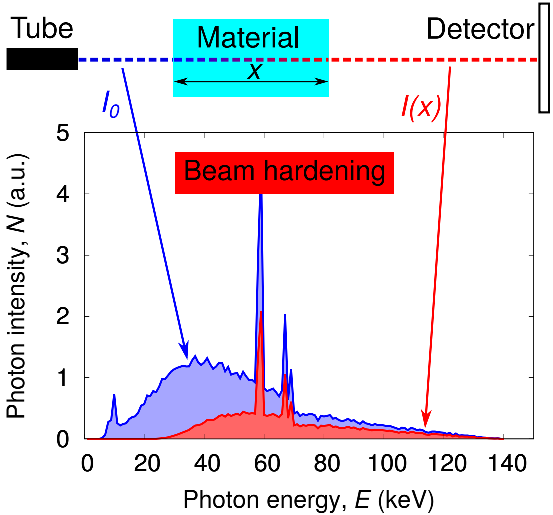
$$\mu \neq \text{const}$$

Thickness: $x = ?$



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

Attenuation of X-rays



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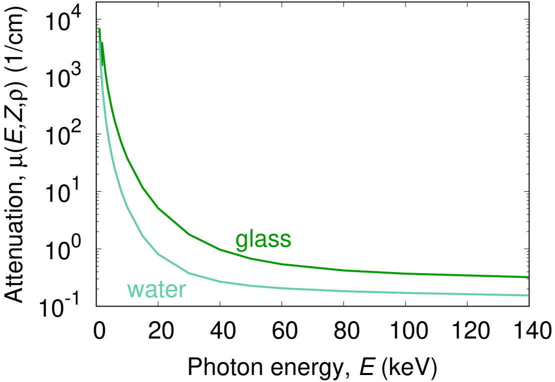

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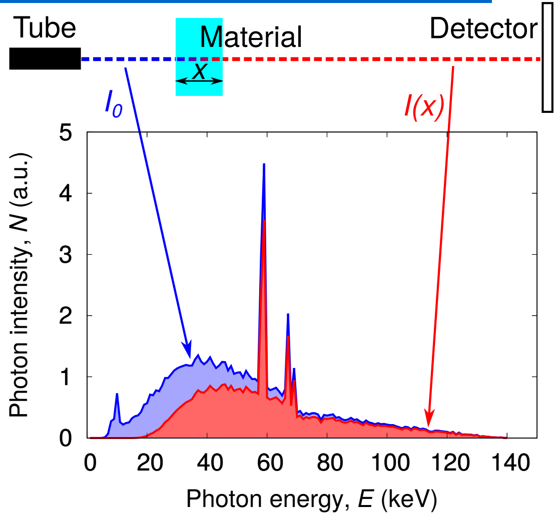
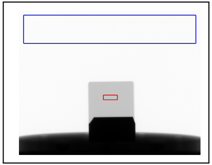
The effective attenuation, μ_{eff}

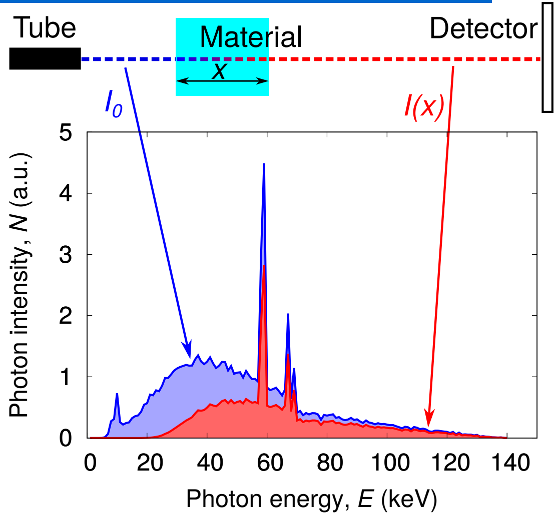


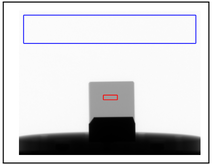


effective attenuation:

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

The effective attenuation, μ_{eff}





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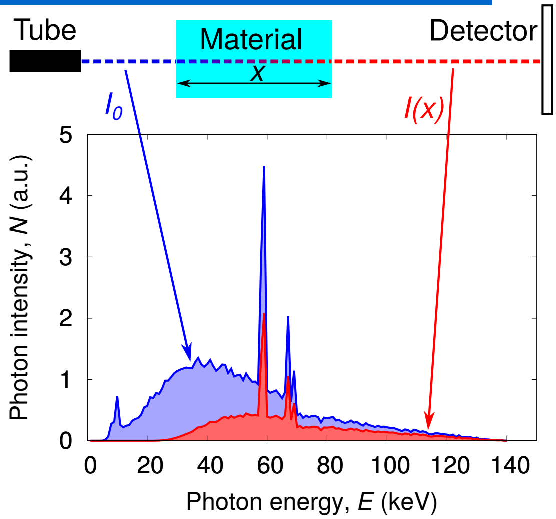

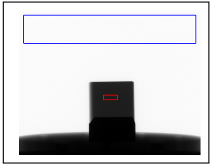

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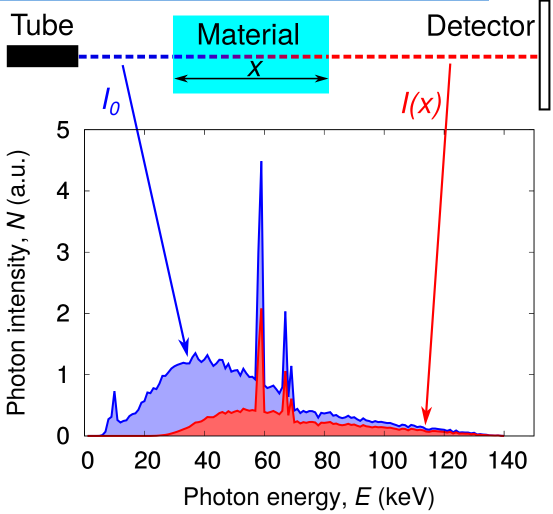
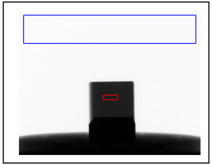
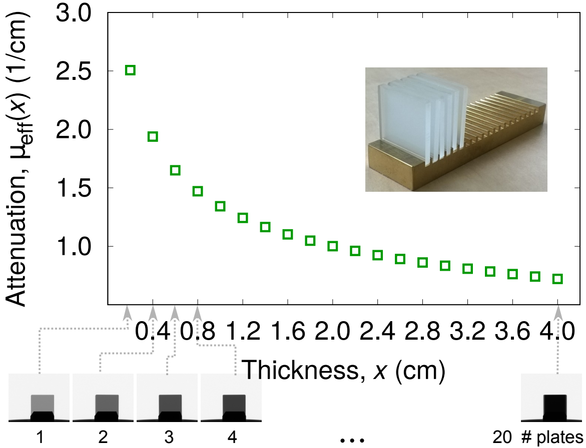




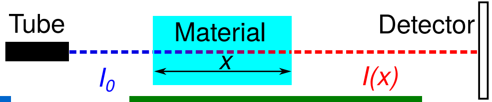
effective attenuation:

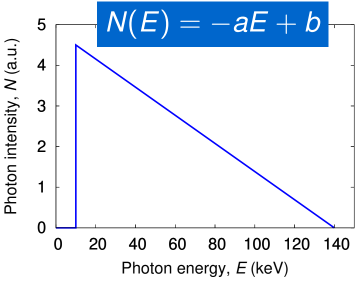
$$I(x) = I_0 \exp(-\mu_{\text{eff}}(x)\, x)$$

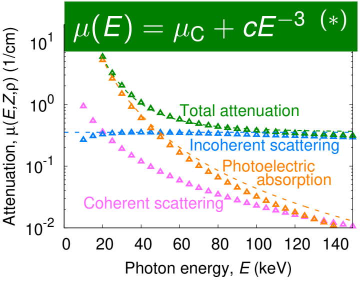
$$\mu_{\text{eff}}(x) = -\frac{1}{x}\frac{I(x)}{I_0}$$

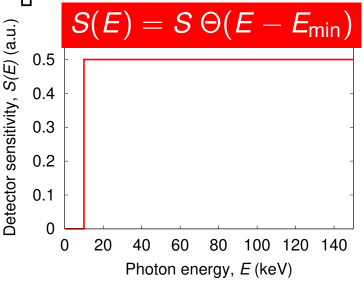


Modeling of μ_{eff}





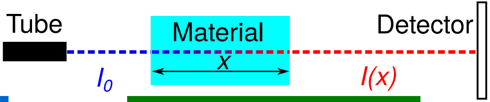




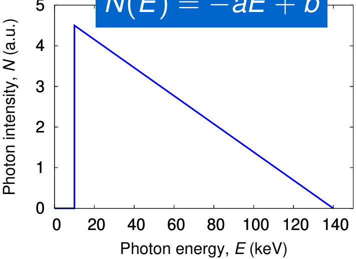
$$I(x) \propto \int N(E) \exp\{-\mu(E, Z, \rho)x\} S(E)\, \mathrm{d}E$$

(∗) XCOM supplied by NIST

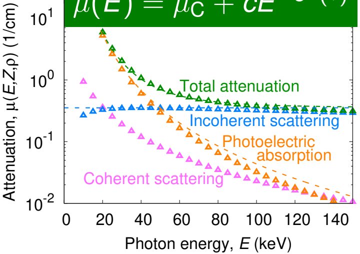
Modeling of μ_{eff}



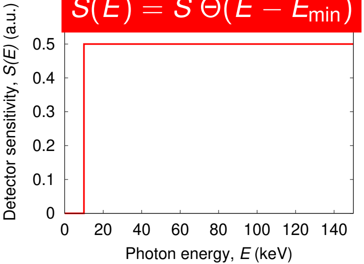
$N(E) = -aE + b$



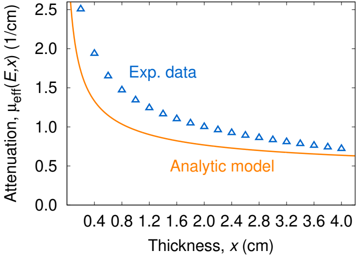
$\mu(E) = \mu_C + cE^{-3} \quad (*)$



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

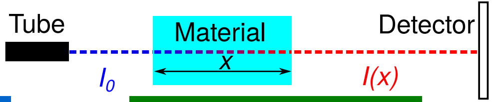


$$I(x) \propto \int N(E) \exp\{-\mu(E, Z, \rho)x\} S(E)\, \mathrm{d}E$$



$(*)$ XCOM supplied by NIST

Modeling of μ_{eff}



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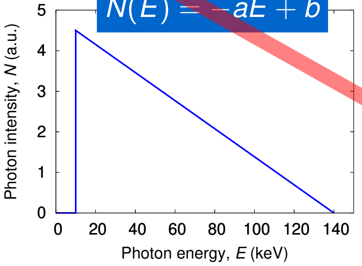

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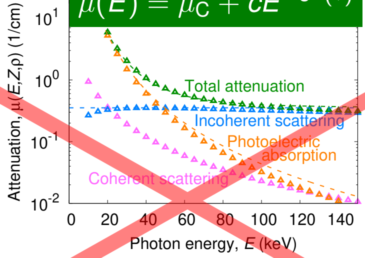

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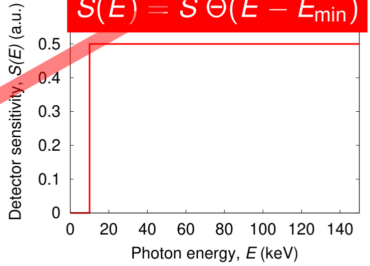

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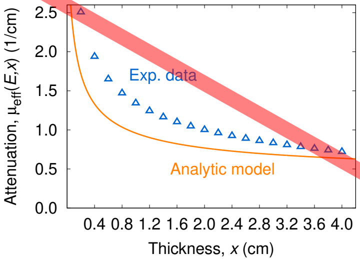

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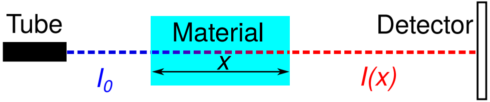
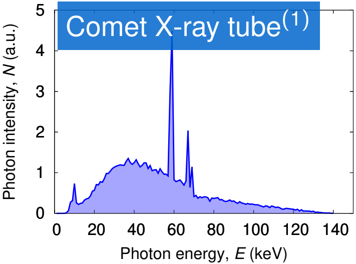
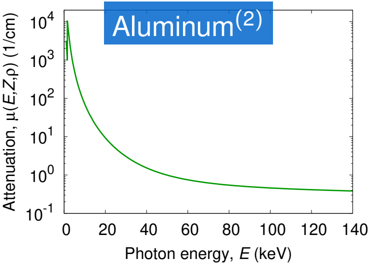
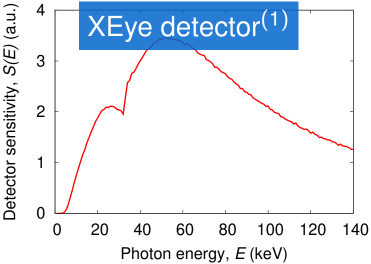
Numerical approx. of μ_{eff}









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

(1) Supplied by Norman Uhlmann, Fraunhofer EZRT

(2) XCOM supplied by NIST

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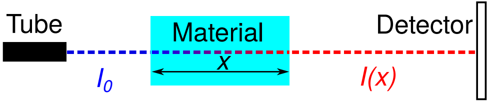

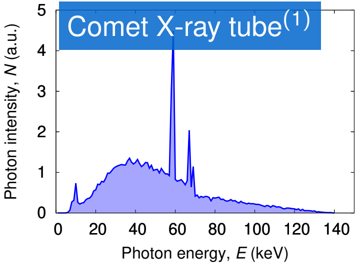

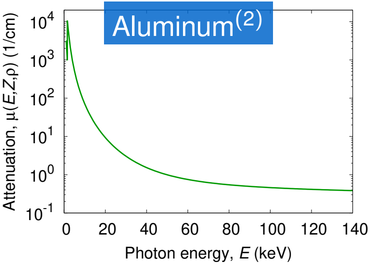

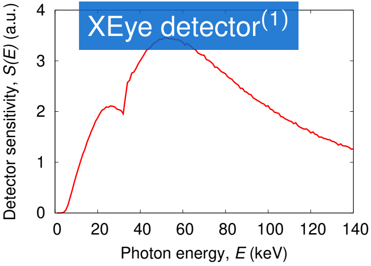

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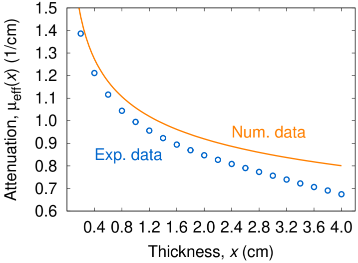

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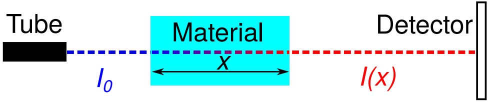

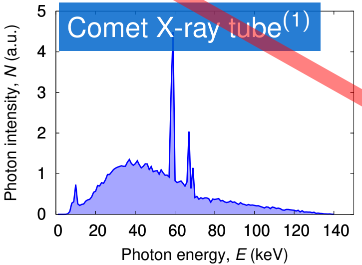

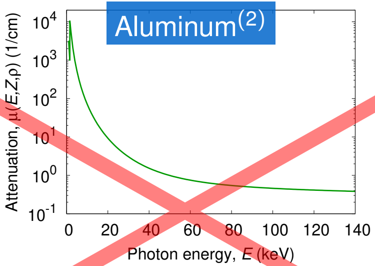

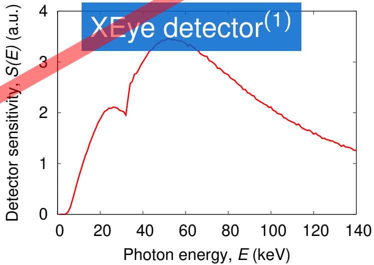

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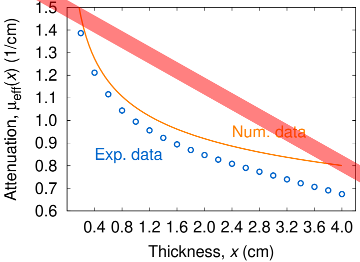

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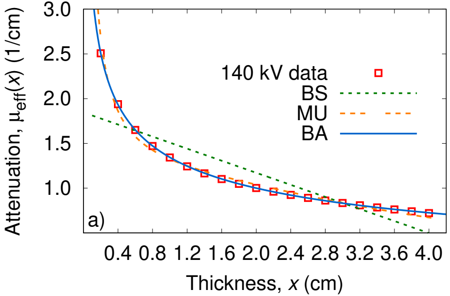
Heuristic model functions for μ_{eff}



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

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)

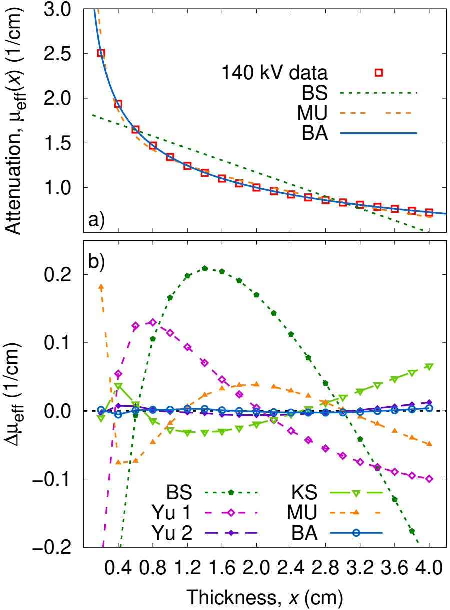
$$\mu_{\text{eff}}(x) = -\frac{1}{x}\ln\left[A + B\exp(-x/C)\right]$$

Mudde *et al.* (2008)

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

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

Heuristic model functions for μ_{eff}



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Baur *et al.* (2019)

(this work)

Universality of
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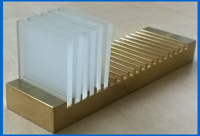

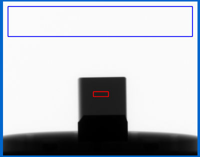

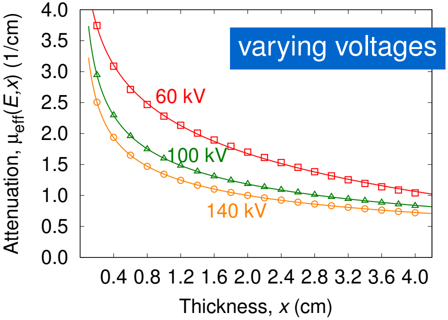

Universality of

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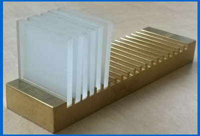
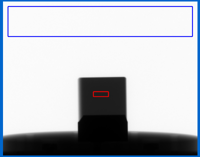
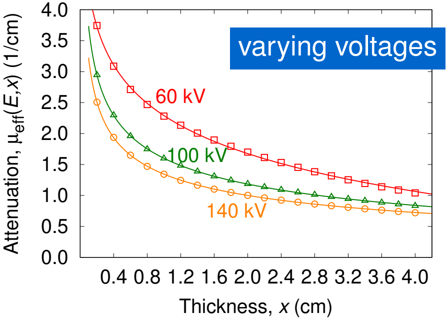
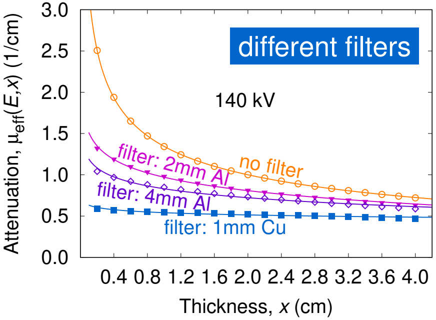
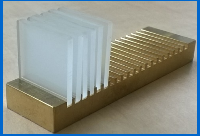


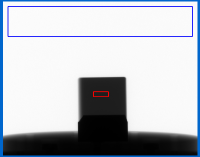


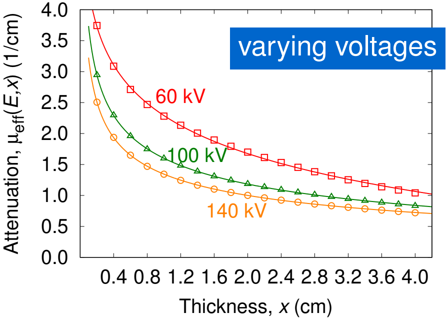


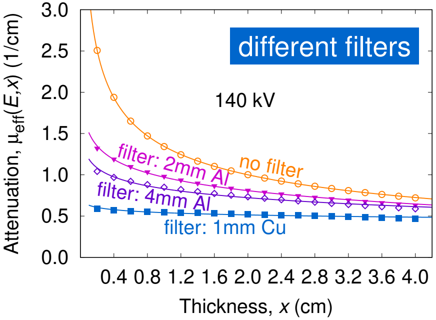


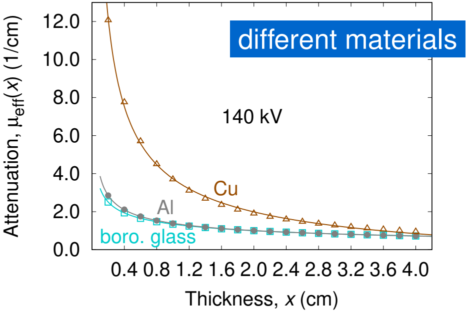
Universality of $\mu_{\mathrm{eff}}(x) = a + \frac{b}{x^{\alpha}}$











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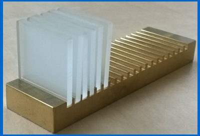
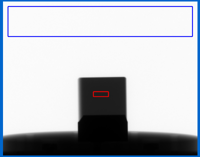
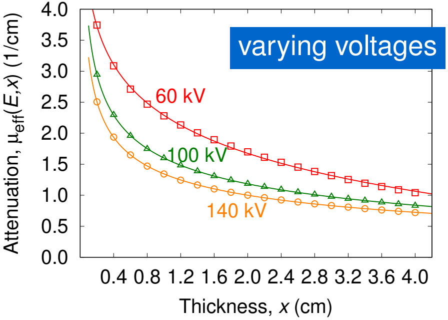
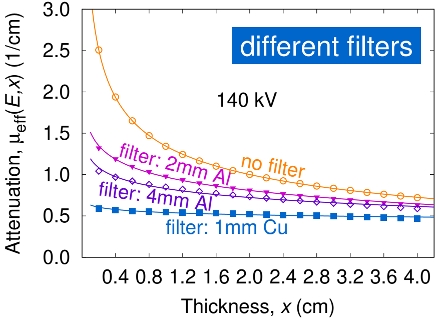
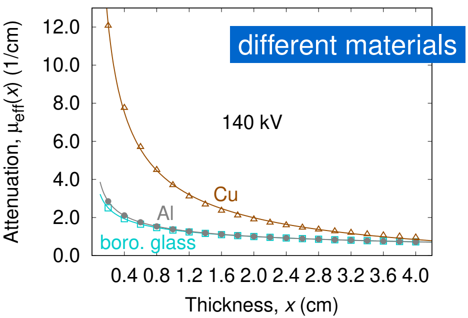
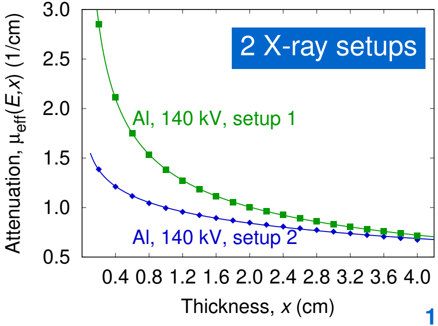












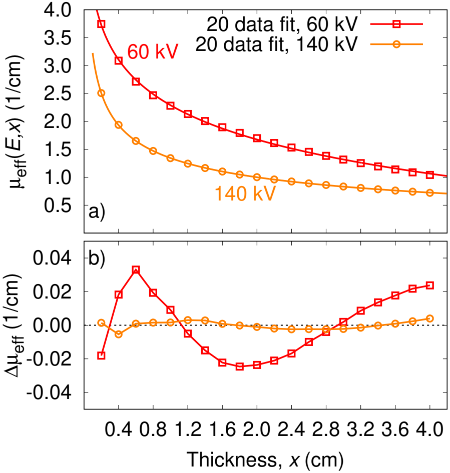
Determining the material thickness x

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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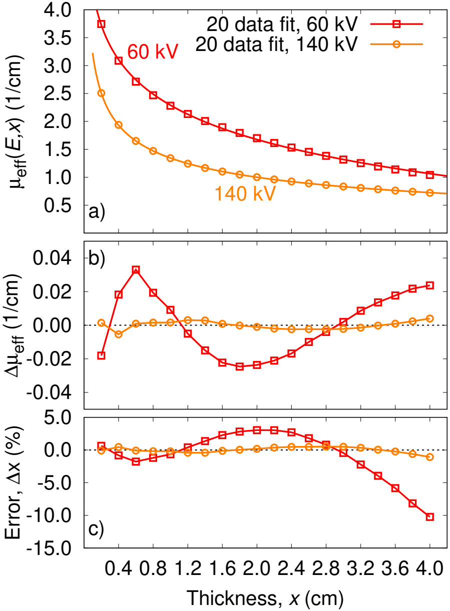
Solve

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

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



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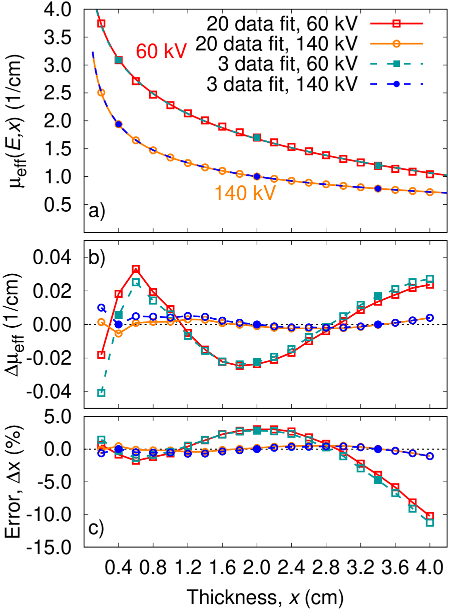
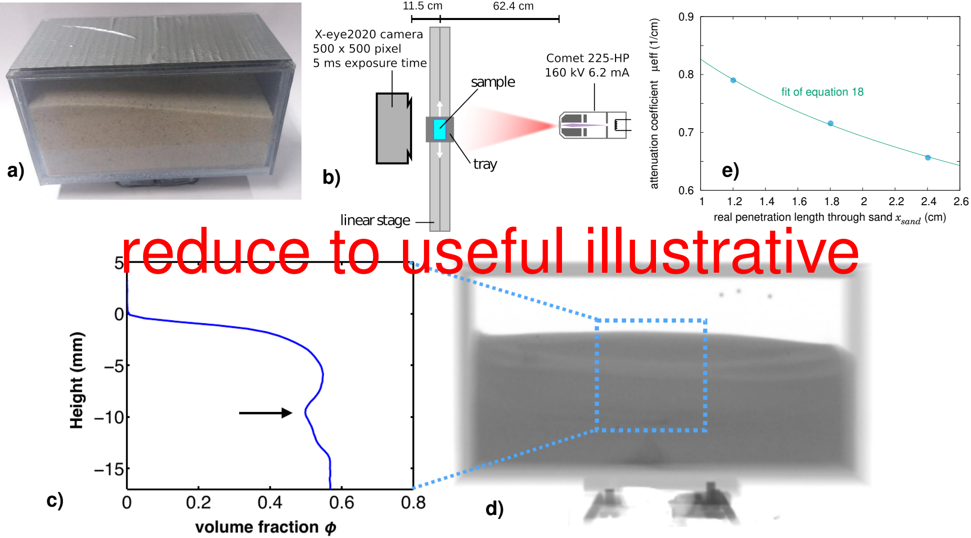


Applications

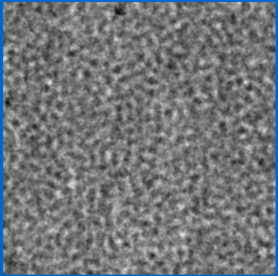


reduce to useful illustrative

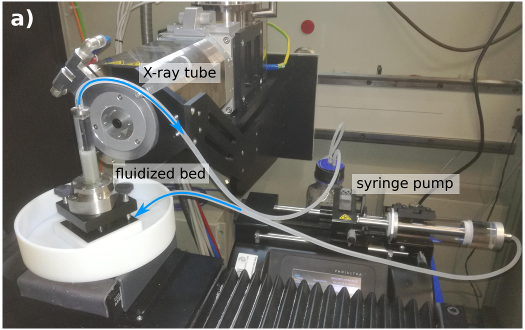
Kollmer *et al* 2020

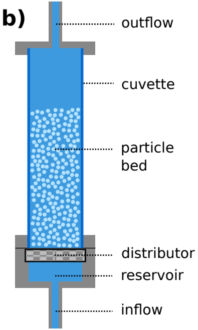
X-ray Digital Fourier Analysis (X-DFA)

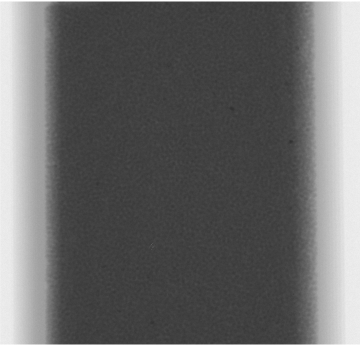
A technique to measure granular dynamics



Experiments

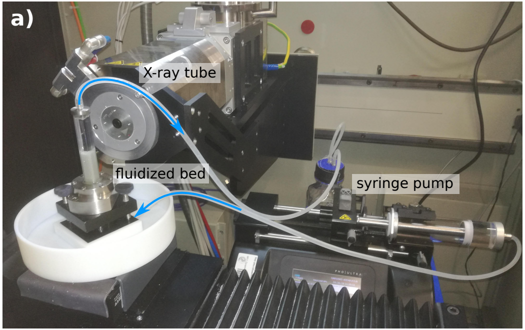


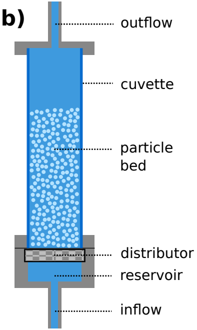


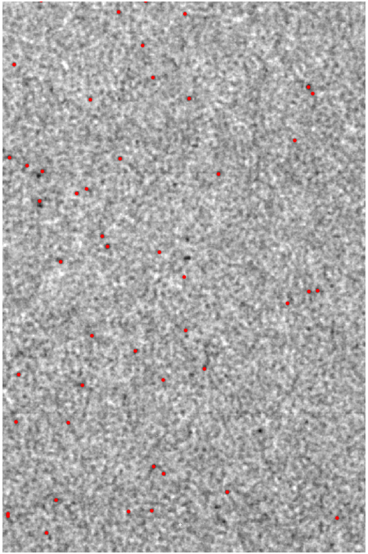


- volume fraction: $0.45 < \Phi < 0.56$
- control dynamics and Φ via pump rate

Experiments







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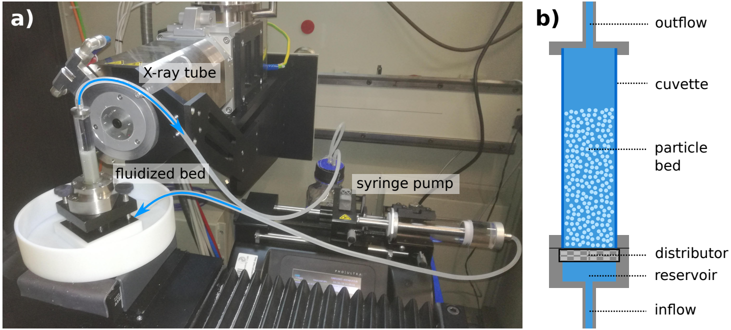

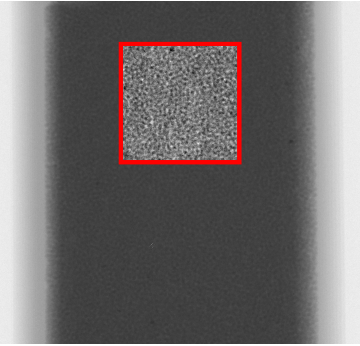

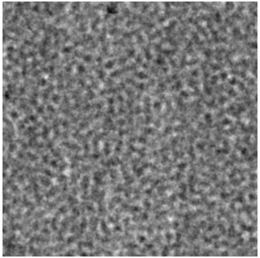

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Differential Dynamic Microscopy (DDM)

	up to now	**this work**
system	dispersion, gels	fluidized bed
particles	colloids	granulate
part. diameter	$< 1\ \mu m$	$\approx 200\ \mu m$
volume fraction	$\Phi \leq 0.33$	$0.45 < \Phi < 0.56$
imaging	light microscope	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

	up to now	this work
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particles	colloids	granulate
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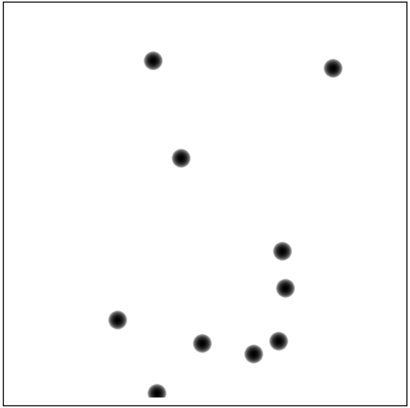
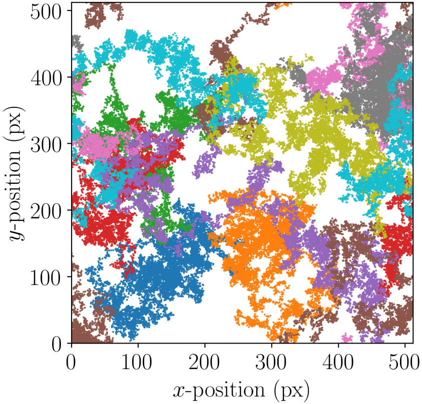
Digital Fourier Analysis of X-Ray Radiograms (X-DFA)

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

Synthetic radiograms



Video 10 Particles



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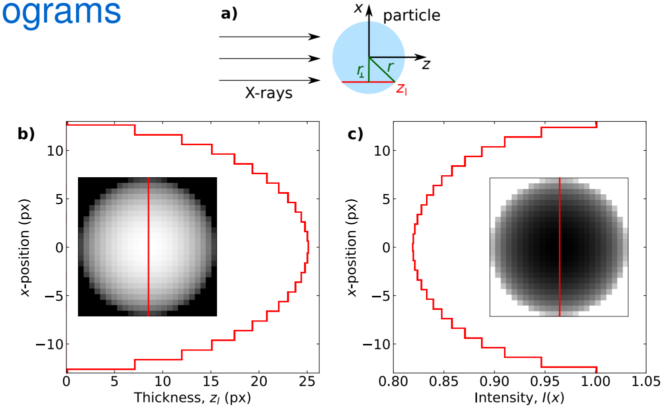

Beer-Lambert

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

Synthetic radiograms

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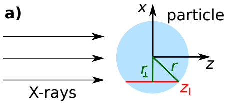

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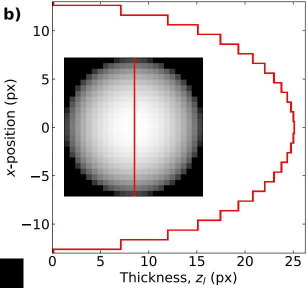
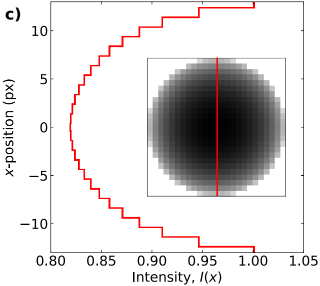
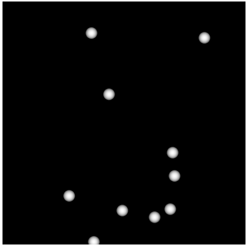


c)




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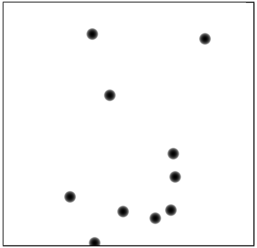
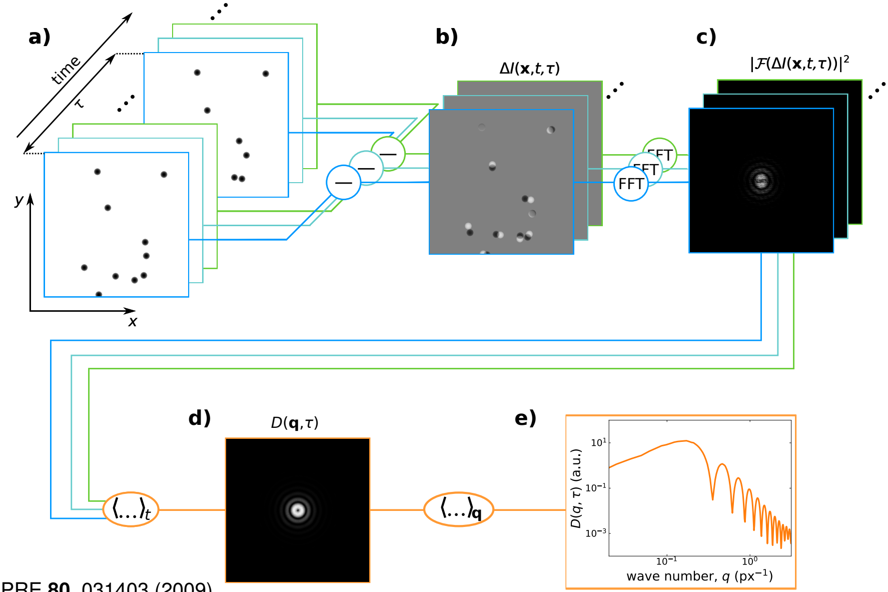


The image structure function $D(\mathbf{q}, \tau)$



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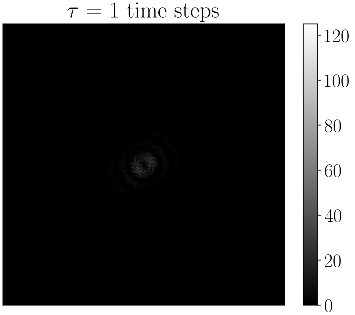

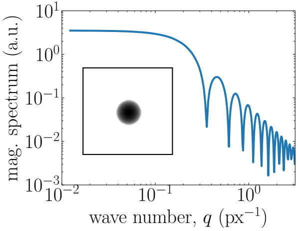

Time averaging: $D(\mathbf{q}, \tau) = \langle |\mathscr{F}(\Delta I)|^2 \rangle_t$

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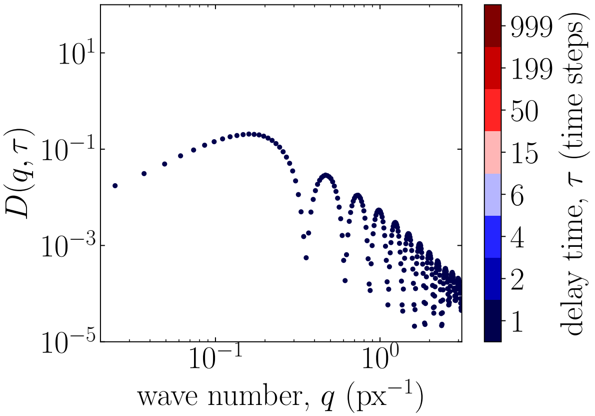

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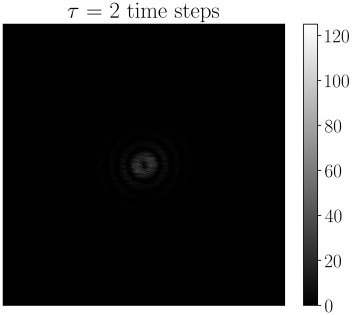

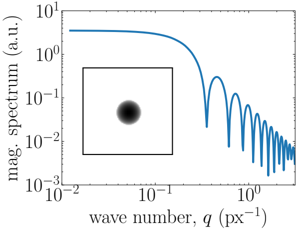

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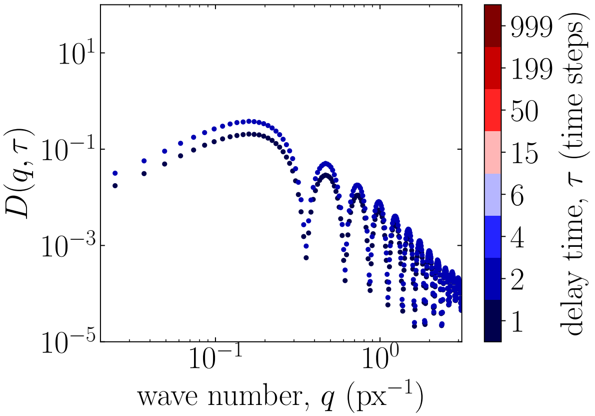

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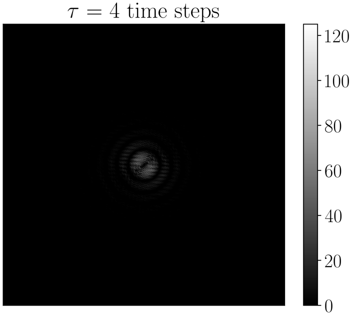

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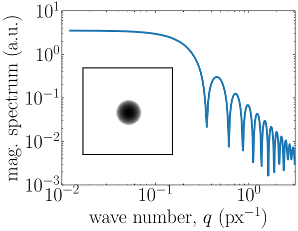

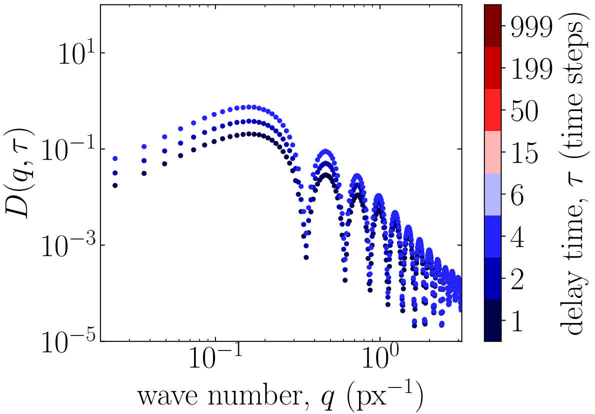

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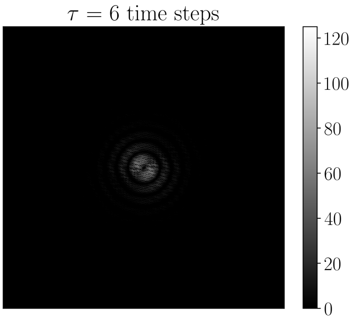

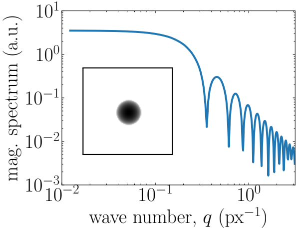

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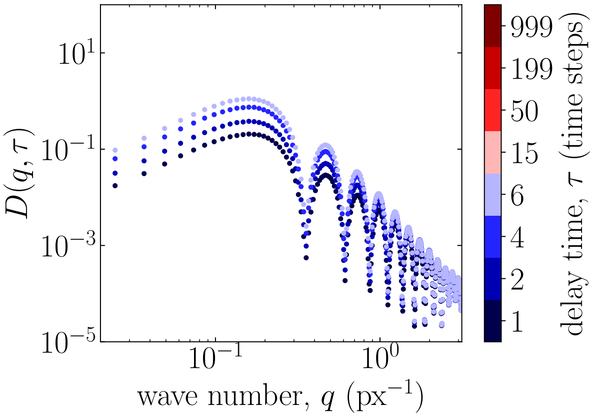

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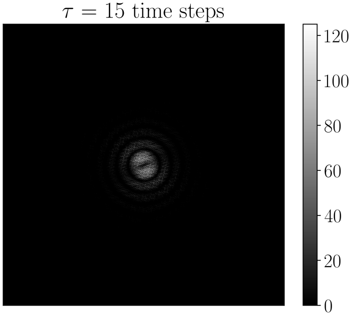

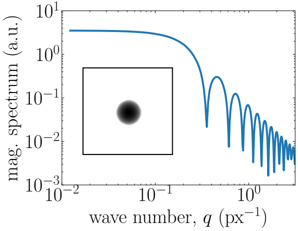

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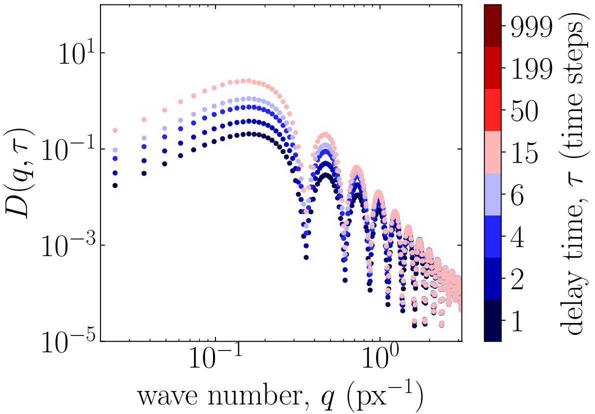

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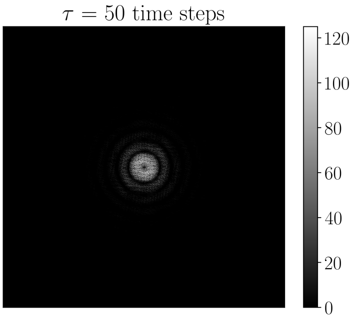

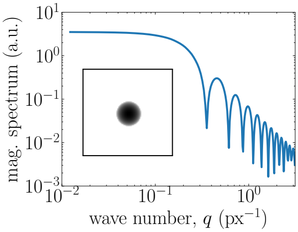

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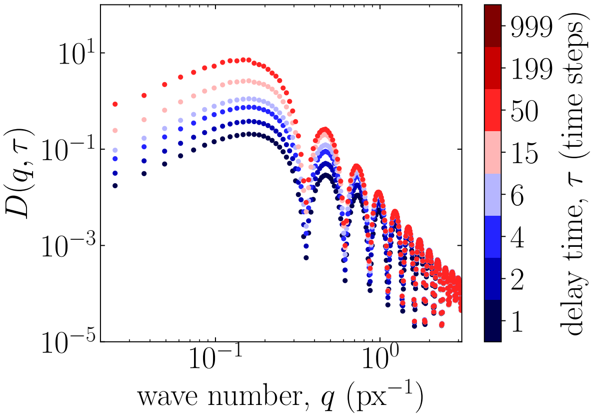

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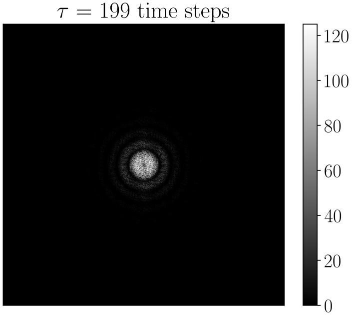

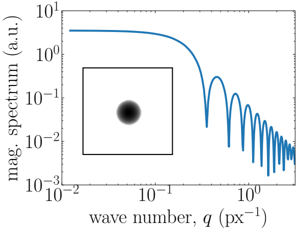

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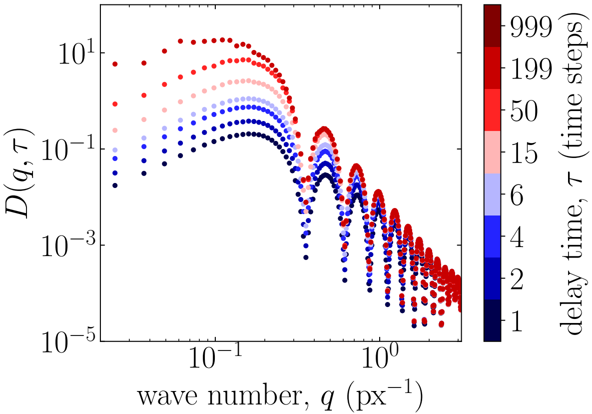

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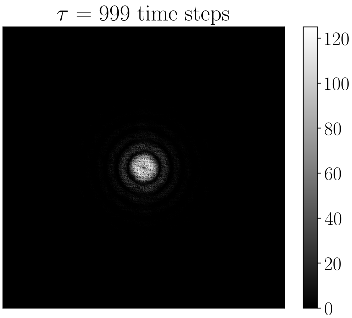

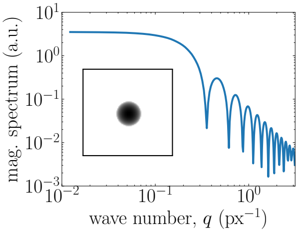

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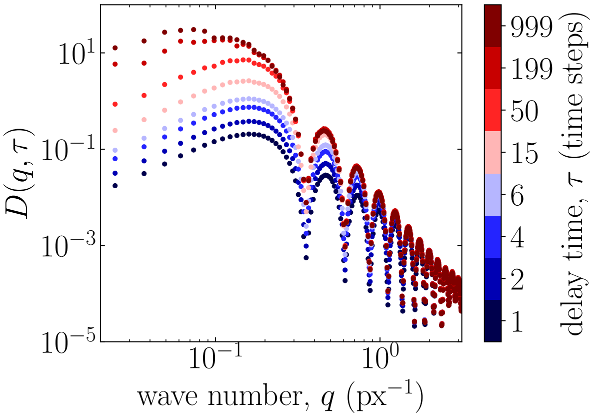

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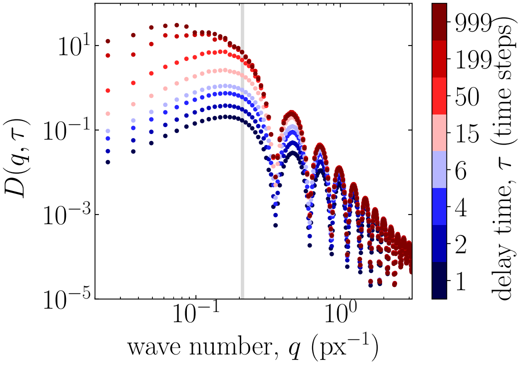
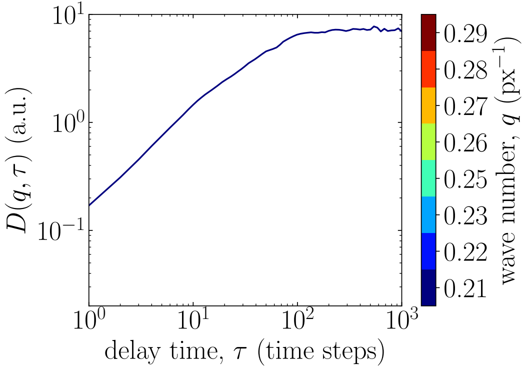
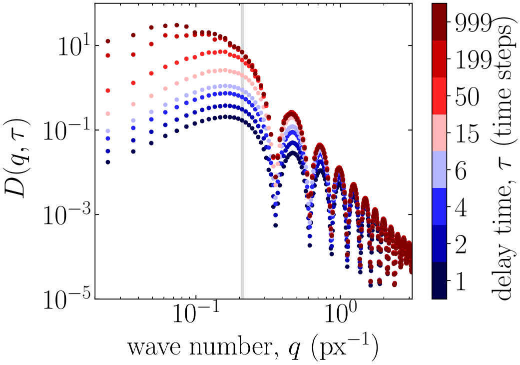
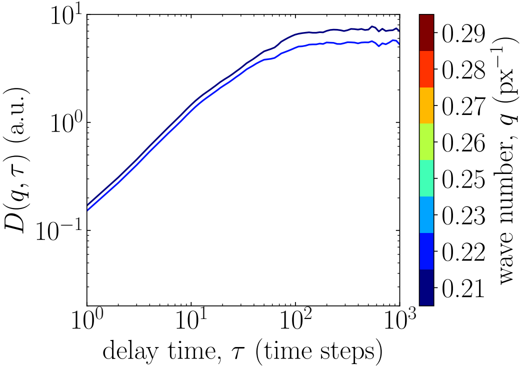


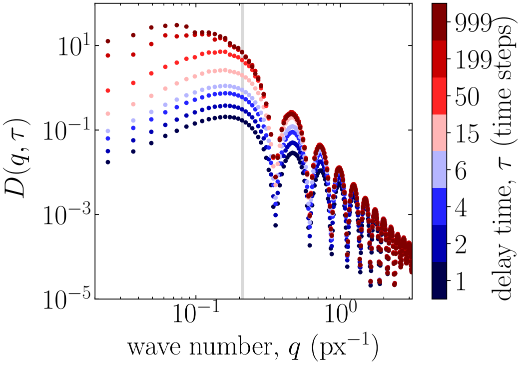


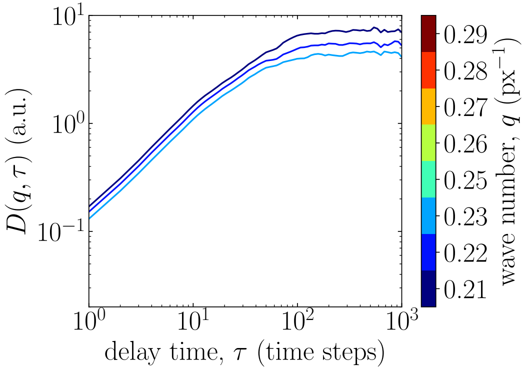
The image structure function $D(q, \tau)$



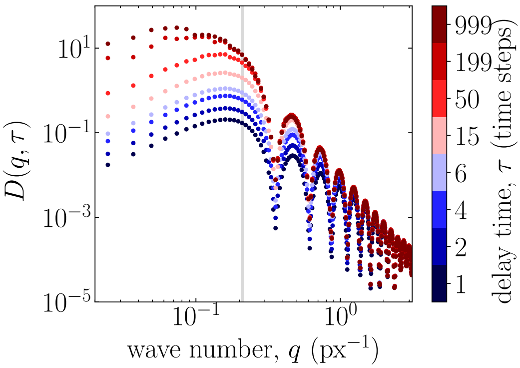


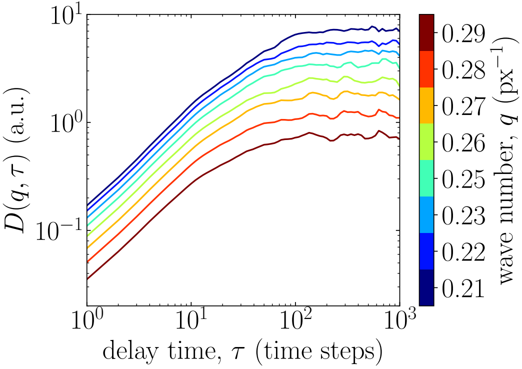
The image structure function $D(q, \tau)$





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

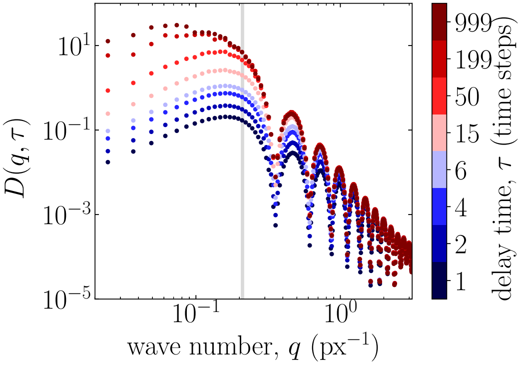


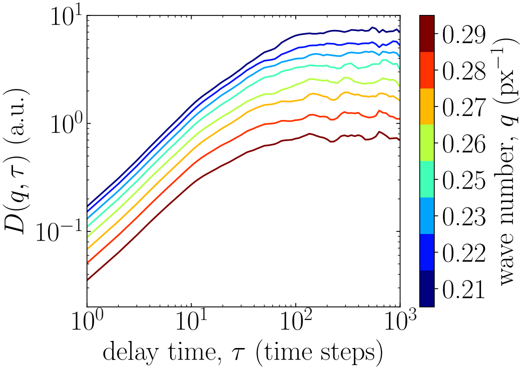


$$D(q,\tau) = \left\langle \left| I(q,t+\tau) - I(q,t) \right|^2 \right\rangle_t$$

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

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





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

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

Linear space invariant imaging

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

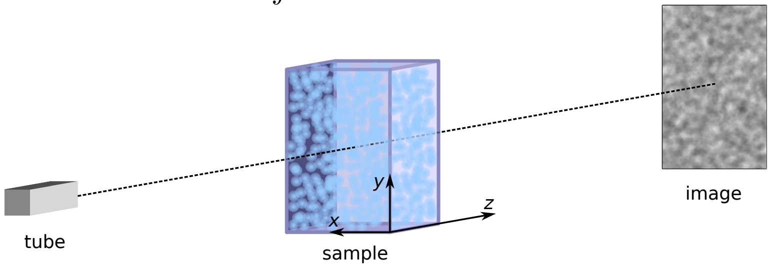
$$g(\mathbf{q}, \tau) = \frac{\langle I^*(\mathbf{q}, t) I(\mathbf{q}, t+\tau) \rangle_t}{\langle |I(\mathbf{q}, t)|^2 \rangle_t}$$

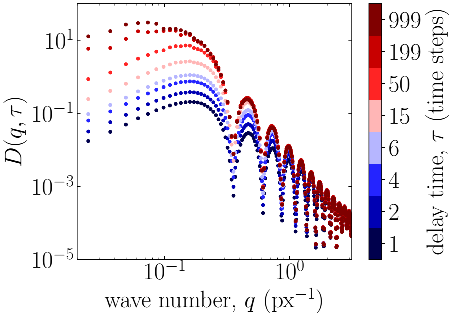
intermediate scattering function

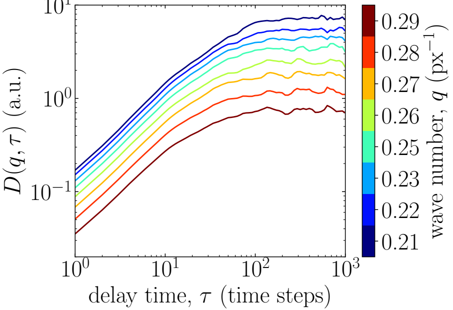
$$f(\mathbf{q}, \tau) = \frac{\langle \rho^*(\mathbf{q}, t) \rho(\mathbf{q}, t+\tau) \rangle_t}{\langle |\rho(\mathbf{q}, t)|^2 \rangle_t}$$

Linear space-invariant imaging:

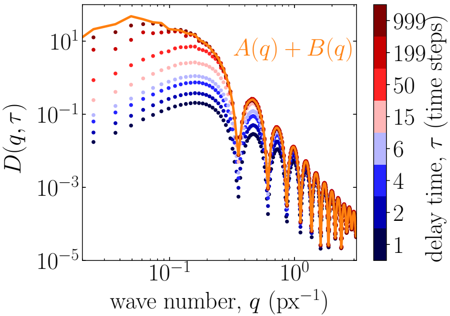
$$I(\mathbf{r}, t) = I_0 + \int \mathrm{d}\mathbf{r}' \, \mathrm{d}z' \, T(\mathbf{r} - \mathbf{r}', -z') c(\mathbf{r}', z', t)$$

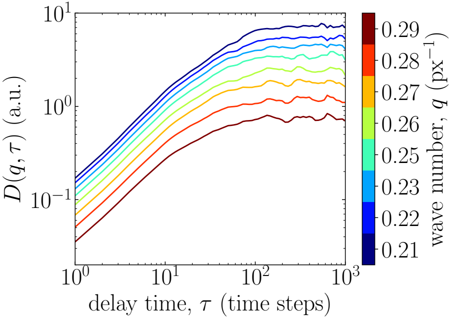






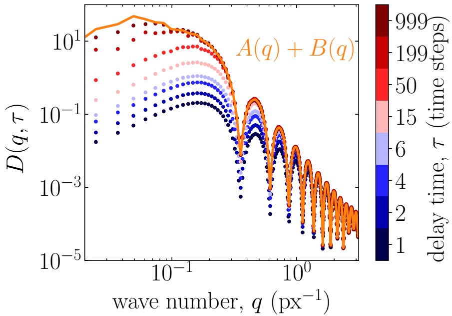
$$
\begin{aligned}
D(q,\tau) &= \left\langle \left| I(q, t+\tau) - I(q,t) \right|^2 \right\rangle_t \\
&= A(q)\left[1 - \underbrace{\frac{\left\langle I^*(q,t)\, I(q,t+\tau)\right\rangle_t}{\left\langle |I(q,t)|^2 \right\rangle_t}}_{\text{image correlation function}}\right] + B(q)
\end{aligned}
$$

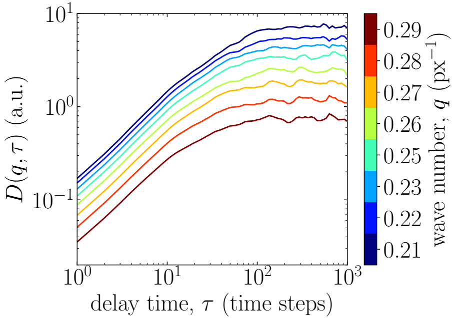




$$D(q,\tau) = \left\langle |I(q,t+\tau) - I(q,t)|^2 \right\rangle_t$$
$$= A(q)\left[1 - \frac{\langle I^*(q,t) I(q,t+\tau)\rangle_t}{\langle |I(q,t)|^2\rangle_t}\right] + B(q)$$

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

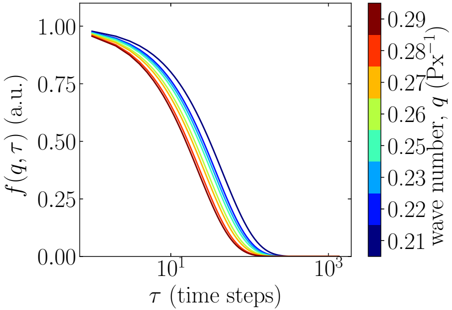




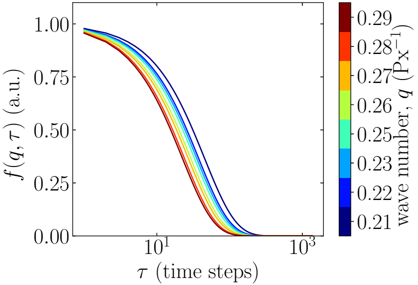
$$D(q,\tau) = \left\langle |I(q,t+\tau) - I(q,t)|^2 \right\rangle_t$$

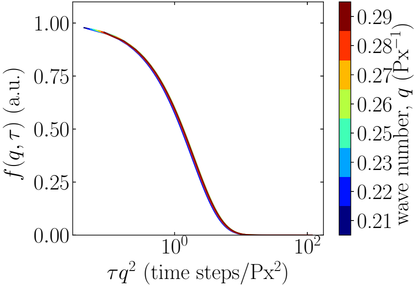
$$= A(q)\left[1 - \frac{\langle I^*(q,t) I(q,t+\tau)\rangle_t}{\langle |I(q,t)|^2\rangle_t}\right] + B(q)$$

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



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

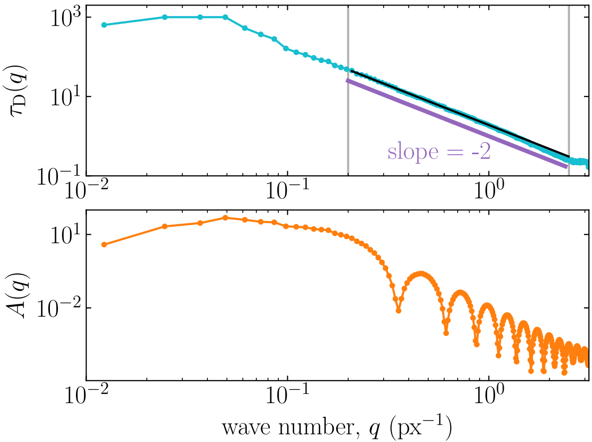




Brownian motion:

$$f(q,\tau) = \exp(-q^2\tau/\tau_\mathrm{D})$$

Accuracy: 2% - 6%

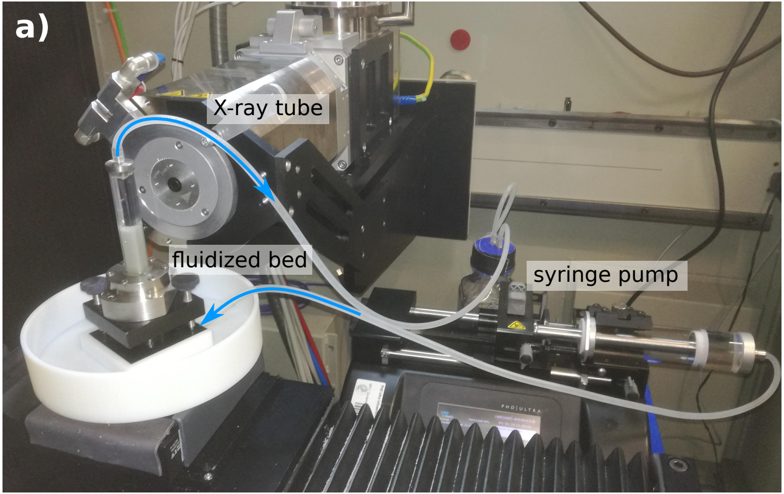


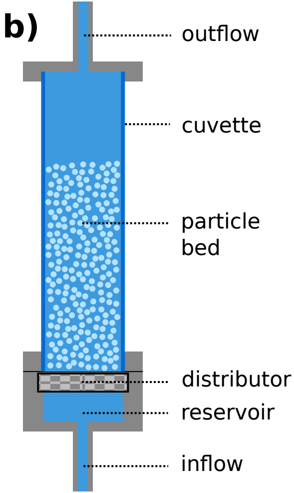
Validating X-DFA on a sedimenting suspension

Measurements on a fluidized bed

Experimental validation: Sedimenting suspension

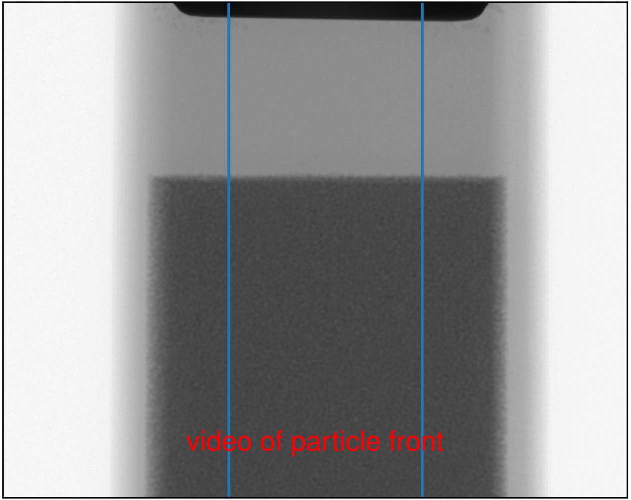
track sedimentation front $\leftrightarrow$ DFA



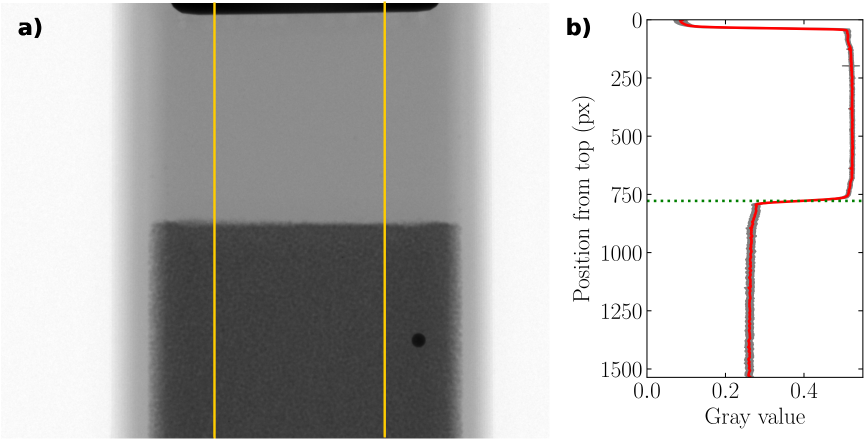


Experimental validation: Sedimenting suspension

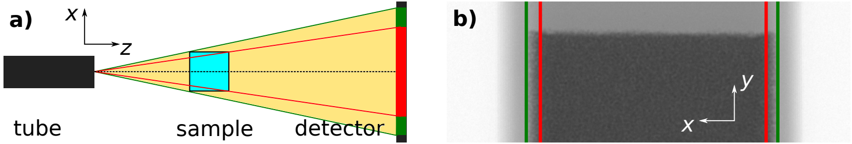
track sedimentation front $\leftrightarrow$ DFA

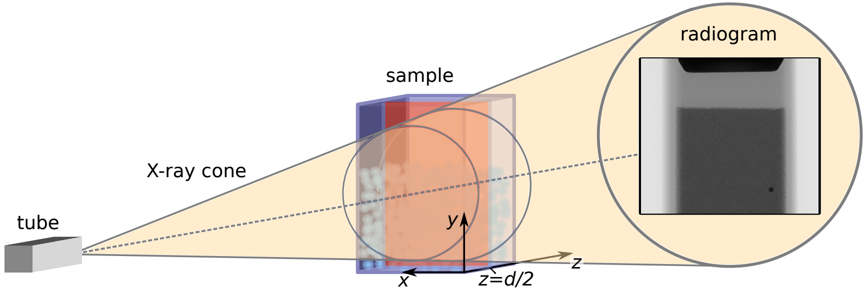


Tracking of particle front

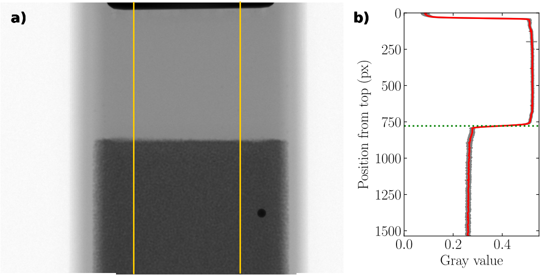


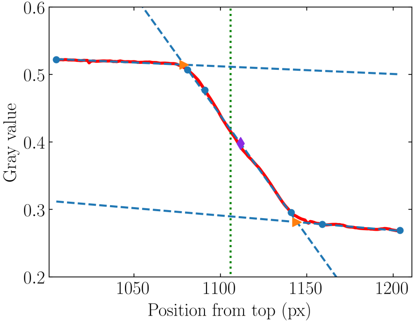
Tracking of particle front

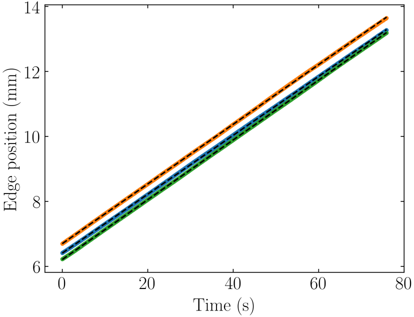




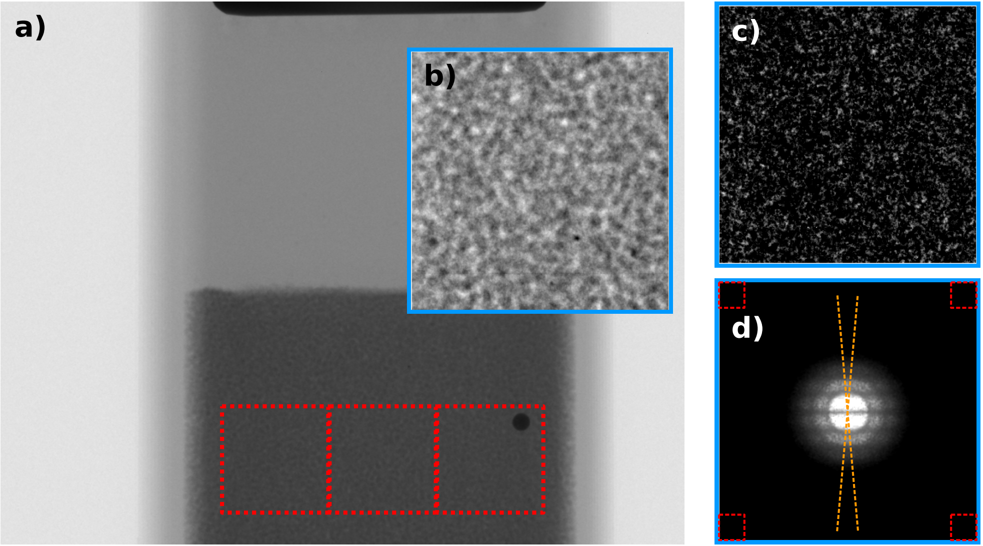
Tracking of particle front



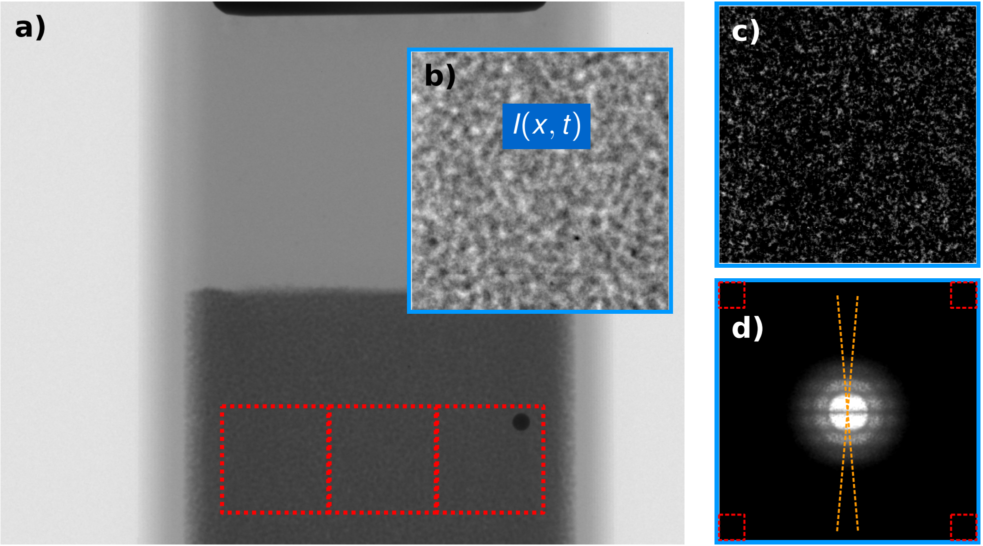




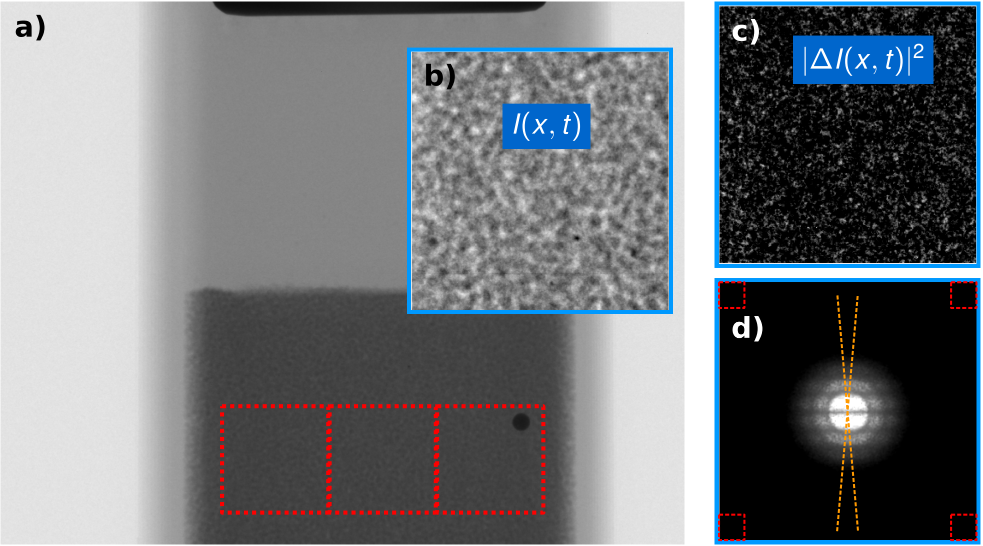
X-DFA for sedimenting particles



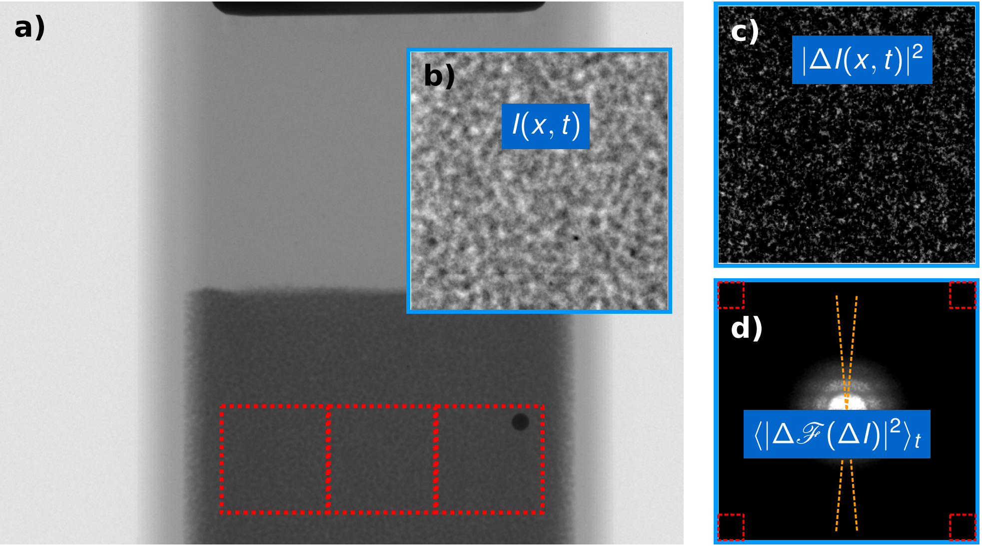
X-DFA for sedimenting particles



X-DFA for sedimenting particles



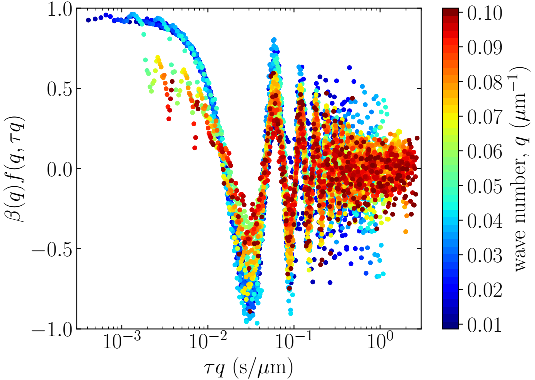
X-DFA for sedimenting particles

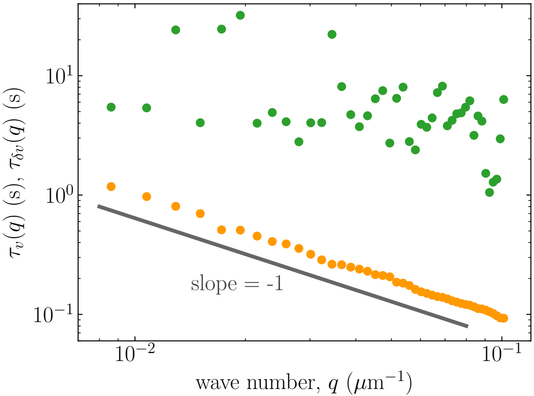


X-DFA for sedimenting particles

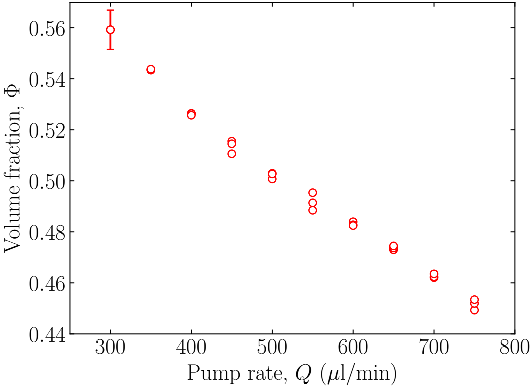
$$f(q,\tau) = \cos(q\langle v_s\rangle\tau)\exp\left(-\frac{1}{2}q^2\delta v^2\tau^2\right)$$

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

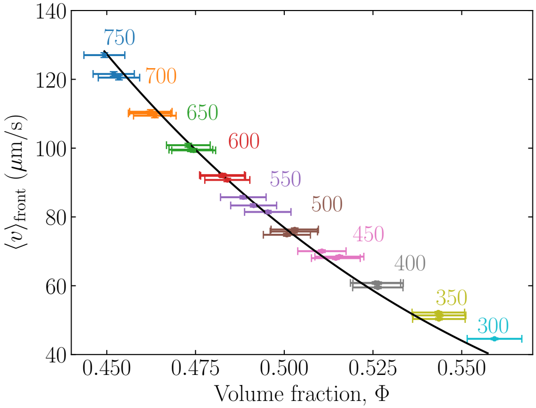




Richardson-Zaki law

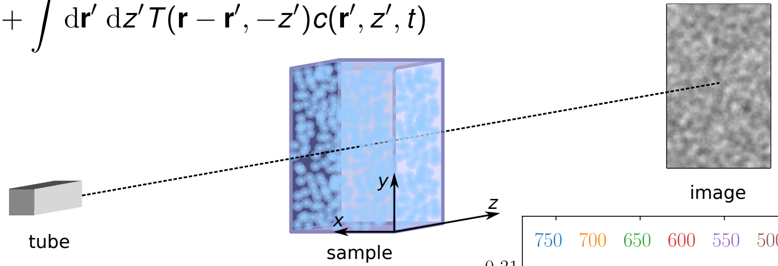


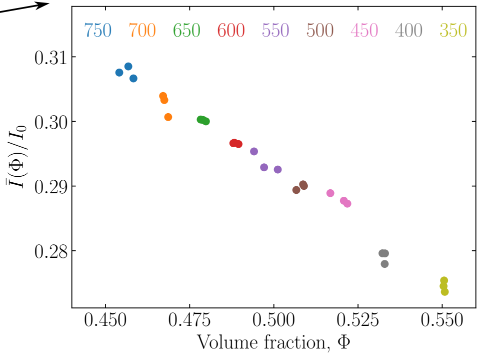
$$\frac{\langle v \rangle_{\mathrm{front}}}{v_{\mathrm{Stokes}}} = (1 - \Phi)^n$$



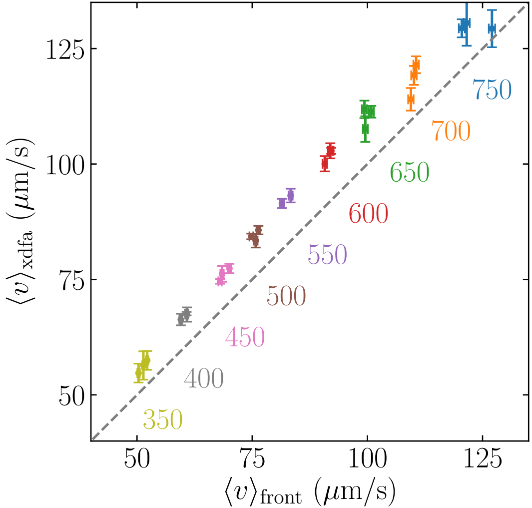
X-DFA: Requirement of linear space invariant imaging

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

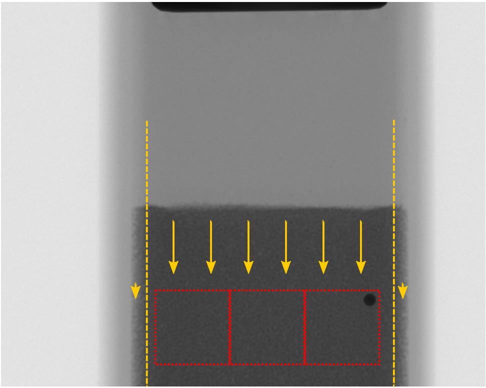




Front tracking vs. X-DFA

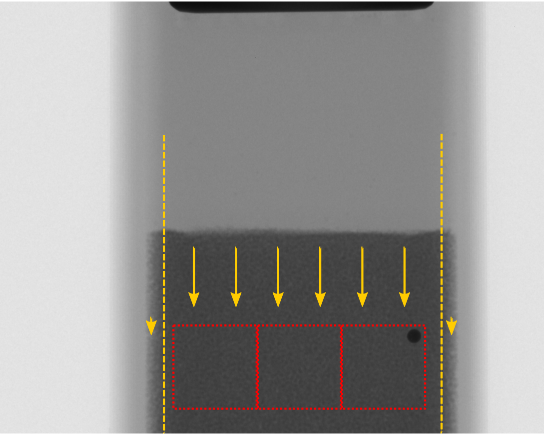


$\langle v \rangle_{\mathrm{xdfa}} > \langle v \rangle_{\mathrm{front}}$ by 9.4%



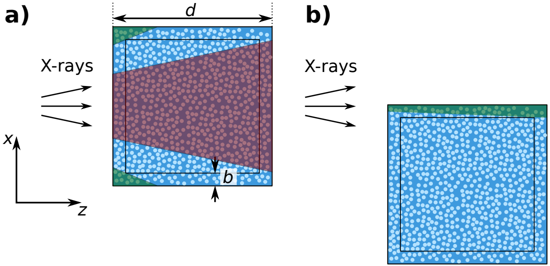
sample video

Estimate width of boundary layer



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

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



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

Thank you for your attention!