

# Package ‘AIUQ’

May 6, 2026

**Type** Package

**Title** Ab Initio Uncertainty Quantification

**Version** 0.5.3

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**Description** Uncertainty quantification and inverse estimation by probabilistic generative models from the beginning of the data analysis. An example is a Fourier basis method for inverse estimation in scattering analysis of microscopy videos. It does not require specifying a certain range of Fourier bases and it substantially reduces computational cost via the generalized Schur algorithm. See the reference: Mengyang Gu, Yue He, Xubo Liu and Yimin Luo (2023), <[doi:10.48550/arXiv.2309.02468](https://doi.org/10.48550/arXiv.2309.02468)>.

**License** GPL (>= 3)

**Encoding** UTF-8

**RoxygenNote** 7.2.3

**Imports** fftwtools (>= 0.9.11), SuperGauss (>= 2.0.3), methods, plot3D (>= 1.4)

**NeedsCompilation** no

**Suggests** knitr, rmarkdown

**VignetteBuilder** knitr

**Repository** CRAN

**Date/Publication** 2024-07-02 07:30:08 UTC

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aniso_SAM	<i>Scattering analysis of microscopy for anisotropic processes</i>
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## Description

Fast parameter estimation in scattering analysis of microscopy for anisotropic processes, using AIUQ method.

## Usage

```
aniso_SAM(
  intensity = NA,
  intensity_str = "T_SS_mat",
  pxsz = 1,
  sz = c(NA, NA),
  mindt = 1,
  AIUQ_thr = c(1, 1),
  model_name = "BM",
  sigma_0_2_ini = NaN,
  param_initial = NA,
  num_optim = 1,
  msd_fn = NA,
  msd_grad_fn = NA,
  num_param = NA,
  uncertainty = FALSE,
  M = 50,
  sim_object = NA,
  msd_truth = NA,
  method = "AIUQ",
  index_q_AIUQ = NA,
  message_out = TRUE,
```

```

    square = FALSE
  )

```

### Arguments

intensity	intensity profile. See 'Details'.
intensity_str	structure of the intensity profile, options from ('SST_array', 'S_ST_mat', 'T_SS_mat'). See 'Details'.
pxsz	size of one pixel in unit of micron, 1 for simulated data
sz	frame size of the intensity profile in x and y directions, number of pixels contained in each frame equals sz_x by sz_y.
mindt	minimum lag time, 1 for simulated data
AIUQ_thr	threshold for wave number selection, numeric vector of two elements with values between 0 and 1. See 'Details'.
model_name	fitted model, options from ('BM', 'OU', 'FBM', 'OU+FBM', 'user_defined'), with Brownian motion as the default model. See 'Details'.
sigma_0_2_ini	initial value for background noise. If NA, use minimum value of absolute square of intensity profile in reciprocal space.
param_initial	initial values for param estimation.
num_optim	number of optimization.
msd_fn	user defined mean squared displacement(MSD) structure, a function of parameters and lag times. NA if model_name is not 'user_defined'.
msd_grad_fn	gradient for user defined mean squared displacement structure. If NA, then numerical gradient will be used for parameter estimation in 'user_defined' model.
num_param	number of parameters need to be estimated in the intermediate scattering function, need to be non-NA value for user_defined' model.
uncertainty	a logical evaluating to TRUE or FALSE indicating whether parameter uncertainty should be computed.
M	number of particles. See 'Details'.
sim_object	NA or an S4 object of class simulation.
msd_truth	true MSD or reference MSD value.
method	methods for parameter estimation, options from ('AIUQ', 'DDM').
index_q_AIUQ	index range for wave number when using AIUQ method. See 'Details'.
message_out	a logical evaluating to TRUE or FALSE indicating whether or not to output the message.
square	a logical evaluating to TRUE or FALSE indicating whether or not to crop the original intensity profile into square image.

## Details

For simulated data using `aniso_simulation` in AIUQ package, intensity will be automatically extracted from `aniso_simulation` class.

By default `intensity_str` is set to `'T_SS_mat'`, a time by space $\times$ space matrix, which is the structure of intensity profile obtained from `aniso_simulation` class. For `intensity_str='SST_array'`, input intensity profile should be a space by space by time array, which is the structure from loading a tif file. For `intensity_str='S_ST_mat'`, input intensity profile should be a space by space $\times$ time matrix.

By default `AIUQ_thr` is set to `c(1, 1)`, uses information from all complete  $q$  rings. The first element affects maximum wave number selected, and second element controls minimum proportion of wave number selected. By setting 1 for the second element, if maximum wave number selected is less than the wave number length, then maximum wave number selected is coerced to use all wave number unless user defined another index range through `index_q_AIUQ`.

If `model_name` equals `'user_defined'`, or NA (will coerced to `'user_defined'`), then `msd_fn` and `num_param` need to be provided for parameter estimation.

Number of particles  $M$  is set to 50 or automatically extracted from simulation class for simulated data using `simulation` in AIUQ package.

By default, using all wave vectors from complete  $q$  ring for both AIUQ, unless user defined index range through `index_q_AIUQ`.

## Value

Returns an S4 object of class `aniso_SAM`.

## Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

## References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

## Examples

```
library(AIUQ)
# Example 1: Estimation for simulated data
set.seed(1)
aniso_sim = aniso_simulation(sz=100, len_t=100, model_name="BM", M=100, sigma_bm=c(0.5, 0.3))
show(aniso_sim)
plot_traj(object=aniso_sim)
aniso_sam = aniso_SAM(sim_object=aniso_sim, model_name="BM", AIUQ_thr = c(0.999, 0))
show(aniso_sam)
plot_MSD(aniso_sam, msd_truth = aniso_sam@msd_truth)
```

---

aniso\_SAM-class      *Anisotropic SAM class*

---

### Description

S4 class for fast parameter estimation in scattering analysis of microscopy for anisotropic processes, using either AIUQ or DDM method.

### Slots

pxsz numeric. Size of one pixel in unit of micron with default value 1.

mindt numeric. Minimum lag time with default value 1.

sz vector. Frame size of the intensity profile in x and y directions, number of pixels contained in each frame equals sz\_x by sz\_y.

len\_t integer. Number of time steps.

len\_q integer. Number of wave vector.

q vector. Wave vector in unit of  $\mu\text{m}^{-1}$ .

d\_input vector. Sequence of lag times.

B\_est\_ini numeric. Estimation of B. This parameter is determined by the noise in the system. See 'References'.

A\_est\_ini vector. Estimation of A(q). Note this parameter is determined by the properties of the imaged material and imaging optics. See 'References'.

I\_o\_q\_2\_ori vector. Absolute square of Fourier transformed intensity profile, ensemble over time.

q\_ori\_ring\_loc\_unique\_index list. List of location index of non-duplicate values for each q ring.

model\_name character. Fitted model, options from ('BM', 'OU', 'FBM', 'OU+FBM', 'user\_defined').

param\_est matrix. Estimated parameters contained in MSD.

sigma\_2\_0\_est vector. Estimated variance of background noise.

msd\_est matrix. Estimated MSD.

uncertainty logical. A logical evaluating to TRUE or FALSE indicating whether parameter uncertainty should be computed.

msd\_truth matrix. True MSD or reference MSD value.

sigma\_2\_0\_truth vector. True variance of background noise, non NA for simulated data using simulation.

param\_truth matrix. True parameters used to construct MSD, non NA for simulated data using aniso\_simulation.

index\_q vector. Selected index of wave vector.

I\_q matrix. Fourier transformed intensity profile with structure 'SS\_T\_mat'.

AIC numeric. Akaike information criterion score.

mle numeric. Maximum log likelihood value.

msd\_x\_lower vector. Lower bound of 95% confidence interval of MSD in x directions.  
 msd\_x\_upper vector. Upper bound of 95% confidence interval of MSD in x directions.  
 msd\_y\_lower vector. Lower bound of 95% confidence interval of MSD in y directions.  
 msd\_y\_upper vector. Upper bound of 95% confidence interval of MSD in y directions.  
 param\_uq\_range matrix. 95% confidence interval for estimated parameters.

### Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

### References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.  
 Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.  
 Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

---

aniso\_simulation

*Simulate anisotropic 2D particle movement*

---

### Description

Simulate anisotropic 2D particle movement from a user selected stochastic process, and output intensity profiles.

### Usage

```
aniso_simulation(
  sz = c(200, 200),
  len_t = 200,
  M = 50,
  model_name = "BM",
  noise = "gaussian",
  I0 = 20,
  Imax = 255,
  pos0 = matrix(NaN, nrow = M, ncol = 2),
  rho = c(0.95, 0.9),
  H = c(0.4, 0.3),
  sigma_p = 2,
  sigma_bm = c(1, 0.5),
  sigma_ou = c(2, 1.5),
  sigma_fbm = c(2, 1.5)
)
```

**Arguments**

sz	frame size of simulated image with default $c(200, 200)$ .
len_t	number of time steps with default 200.
M	number of particles with default 50.
model_name	stochastic process simulated, options from ('BM', 'OU', 'FBM', 'OU+FBM'), with default 'BM'.
noise	background noise, options from ('uniform', 'gaussian'), with default 'gaussian'.
I0	background intensity, value between 0 and 255, with default 20.
Imax	maximum intensity at the center of the particle, value between 0 and 255, with default 255.
pos0	initial position for M particles, matrix with dimension M by 2.
rho	correlation between successive step and previous step in O-U process, in x, y-directions. A vector of length 2 with values between 0 and 1, default $c(0.95, 0.9)$ .
H	Hurst parameter of fractional Brownian Motion, in x, y-directions. A vector of length 2, value between 0 and 1, default $c(0.4, 0.3)$ .
sigma_p	radius of the spherical particle ( $3\sigma_p$ ), with default 2.
sigma_bm	distance moved per time step of Brownian Motion, in x,y-directions. A vector of length 2 with default $c(1, 0.5)$ .
sigma_ou	distance moved per time step of Ornstein–Uhlenbeck process, in x, y-directions. A vector of length 2 with default $c(2, 1.5)$ .
sigma_fbm	distance moved per time step of fractional Brownian Motion, in x, y-directions. A vector of length 2 with default $c(2, 1.5)$ .

**Value**

Returns an S4 object of class `anisotropic_simulation`.

**Author(s)**

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

**References**

- Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.
- Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.
- Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

**Examples**

```

library(AIUQ)
# -----
# Example 1: Simple diffusion for 200 images with
#           200 by 200 pixels and 50 particles
# -----
aniso_sim_bm = aniso_simulation()
show(aniso_sim_bm)

# -----
# Example 2: Simple diffusion for 100 images with
#           100 by 100 pixels and slower speed
# -----
aniso_sim_bm = aniso_simulation(sz=100,len_t=100,sigma_bm=c(0.5,0.1))
show(aniso_sim_bm)

# -----
# Example 3: Ornstein-Uhlenbeck process
# -----
aniso_sim_ou = aniso_simulation(model_name="OU")
show(aniso_sim_ou)

```

---

aniso\_simulation-class

*Anisotropic simulation class*

---

**Description**

S4 class for anisotropic 2D particle movement simulation.

**Details**

intensity should has structure 'T\_SS\_mat', matrix with dimension len\_t by sz×sz.

pos should be the position matrix with dimension M×len\_t. See [bm\\_particle\\_intensity](#), [ou\\_particle\\_intensity](#), [fbm\\_particle\\_intensity](#), [fbm\\_ou\\_particle\\_intensity](#).

**Slots**

sz vector. Frame size of the intensity profile, number of pixels contained in each frame equals sz[1] by sz[2].

len\_t integer. Number of time steps.

noise character. Background noise, options from ('uniform','gaussian').

model\_name character. Simulated stochastic process, options from ('BM','OU','FBM','OU+FBM').

M integer. Number of particles.

pxsz numeric. Size of one pixel in unit of micron, 1 for simulated data.

mindt numeric. Minimum lag time, 1 for simulated data.

pos matrix. Position matrix for particle trajectory, see 'Details'.

intensity matrix. Filled intensity profile, see 'Details'.

num\_msd matrix. Numerical mean squared displacement (MSD).

param matrix. Parameters used to construct MSD.

theor\_msd matrix. Theoretical MSD.

sigma\_2\_0 vector. Variance of background noise.

### Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

### References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

---

get\_dqt

*Compute observed dynamic image structure function*

---

### Description

Compute observed dynamic image structure function (Dqt) using object of SAM class.

### Usage

```
get_dqt(object, index_q = NA)
```

### Arguments

object	an S4 object of class SAM
index_q	wavevector range used for computing Dqt

### Value

A matrix of observed dynamic image structure function with dimension len\_q by len\_t-1.

### Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

## References

- Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.
- Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.
- Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

## Examples

```
## Not run:
library(AIUQ)
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
Dqt = get_dqt(object=sam)

## End(Not run)
```

---

get\_isf

*Compute empirical intermediate scattering function*

---

## Description

Compute empirical intermediate scattering function (ISF) using object of SAM class.

## Usage

```
get_isf(object, index_q = NA, msd_truth = NA)
```

## Arguments

object	an S4 object of class SAM
index_q	wavevector range used for computing ISF
msd_truth	true or reference MSD

## Value

A matrix of empirical intermediate scattering function with dimension len\_q by len\_t-1.

## Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

## References

- Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.
- Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.
- Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

## Examples

```
## Not run:
library(AIUQ)
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
ISF = get_isf(object=sam)

## End(Not run)
```

---

modeled\_dqt

---

*Compute modeled dynamic image structure function*


---

## Description

Compute modeled dynamic image structure function (Dqt) using object of SAM class.

## Usage

```
modeled_dqt(object, index_q = NA, uncertainty = FALSE)
```

## Arguments

object	an S4 object of class SAM
index_q	wavevector range used for computing Dqt
uncertainty	logic evaluation

## Value

A matrix of modeled dynamic image structure function with dimension len\_q by len\_t-1.

## Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

## References

- Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.
- Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.
- Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

## Examples

```
library(AIUQ)
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
modeled_Dqt = modeled_dqt(object=sam)
```

---

modeled\_isf

*Compute modeled intermediate scattering function*

---

## Description

Compute modeled intermediate scattering function (ISF) using object of SAM class.

## Usage

```
modeled_isf(object, index_q = NA)
```

## Arguments

object	an S4 object of class SAM
index_q	wavevector range used for computing ISF

## Value

A matrix of modeled intermediate scattering function with dimension len\_q by len\_t-1.

## Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

## References

- Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.
- Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.
- Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

## Examples

```
library(AIUQ)
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
modeled_ISF = modeled_isf(object=sam)
```

---

plot_intensity	<i>Plot 2D intensity</i>
----------------	--------------------------

---

## Description

Function to plot 2D intensity profile for a certain frame, default is to plot the first frame. Input can be a matrix (2D) or an array (3D).

## Usage

```
plot_intensity(
  intensity,
  intensity_str = "T_SS_mat",
  frame = 1,
  sz = NA,
  title = NA,
  color = FALSE
)
```

## Arguments

intensity	intensity profile
intensity_str	structure of the intensity profile, options from ('SST_array', 'S_ST_mat', 'T_SS_mat', 'SS_T_mat'). See 'Details'.
frame	frame index
sz	frame size of simulated image with default c(200, 200).
title	main title of the plot. If NA, title is "intensity profile for frame n" with n being the frame index in frame.
color	a logical evaluating to TRUE or FALSE indicating whether a colorful plot is generated

**Details**

By default `intensity_str` is set to `'T_SS_mat'`, a time by  $\text{space} \times \text{space}$  matrix, which is the structure of intensity profile obtained from `simulation` class. For `intensity_str='SST_array'`, input intensity profile should be a space by space by time array, which is the structure from loading a tif file. For `intensity_str='S_ST_mat'`, input intensity profile should be a space by  $\text{space} \times \text{time}$  matrix. For `intensity_str='SS_T_mat'`, input intensity profile should be a  $\text{space} \times \text{space}$  by time matrix.

**Value**

2D plot in gray scale (or with color) of selected frame.

**Author(s)**

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

**Examples**

```
library(AIUQ)
sim_bm = simulation(sz=100, len_t=100, sigma_bm=0.5)
show(sim_bm)
plot_intensity(sim_bm@intensity, sz=sim_bm@sz)
```

---

plot\_MSD

*Plot estimated MSD with uncertainty from SAM class*

---

**Description**

Function to plot estimated MSD with uncertainty from SAM class, versus true mean squared displacement(MSD) or given reference values.

**Usage**

```
plot_MSD(object, msd_truth = NA, title = NA, log10 = TRUE)
```

**Arguments**

<code>object</code>	an S4 object of class SAM
<code>msd_truth</code>	a vector/matrix of true MSD or reference MSD value, default is NA
<code>title</code>	main title of the plot. If NA, title is "model_name" with <code>model_name</code> being a field in SAM class representing fitted model.
<code>log10</code>	a logical evaluating to TRUE or FALSE indicating whether a plot in log10 scale is generated

**Value**

A plot of estimated MSD with uncertainty versus truth/reference values.

**Author(s)**

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

**References**

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

**Examples**

```
library(AIUQ)

## Simulate BM and get estimated parameters with uncertainty using BM model
# Simulation
set.seed(1)
sim_bm = simulation(sz=100, len_t=100, sigma_bm=0.5)
show(sim_bm)

# AIUQ method: fitting using BM model
sam = SAM(sim_object=sim_bm, uncertainty=TRUE, AIUQ_thr=c(0.999, 0))
show(sam)

plot_MSD(object=sam, msd_truth=sam@msd_truth) #in log10 scale
plot_MSD(object=sam, msd_truth=sam@msd_truth, log10=FALSE) #in real scale
```

---

plot\_traj

*Plot 2D particle trajectory*

---

**Description**

Function to plot the particle trajectory after the simulation class has been constructed.

**Usage**

```
plot_traj(object, title = NA)
```

**Arguments**

object	an S4 object of class simulation
title	main title of the plot. If NA, title is "model_name with M particles" with model_name and M being field in simulation class.

**Value**

2D plot of particle trajectory for a given simulation from simulation class.

**Author(s)**

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

**Examples**

```
library(AIUQ)
sim_bm = simulation(sz=100,len_t=100,sigma_bm=0.5)
show(sim_bm)
plot_traj(sim_bm)
```

---

SAM

*Scattering analysis of microscopy*

---

**Description**

Fast parameter estimation in scattering analysis of microscopy, using either AIUQ or DDM method.

**Usage**

```
SAM(
  intensity = NA,
  intensity_str = "T_SS_mat",
  pxsz = 1,
  sz = c(NA, NA),
  mindt = 1,
  AIUQ_thr = c(1, 1),
  model_name = "BM",
  sigma_0_2_ini = NaN,
  param_initial = NA,
  num_optim = 1,
  msd_fn = NA,
  msd_grad_fn = NA,
  num_param = NA,
  uncertainty = FALSE,
  M = 50,
  sim_object = NA,
  msd_truth = NA,
  method = "AIUQ",
  index_q_AIUQ = NA,
  index_q_DDM = NA,
  message_out = TRUE,
  A_neg = "abs",
  square = FALSE,
  output_dqt = FALSE,
  output_isf = FALSE,
  output_modeled_isf = FALSE,
  output_modeled_dqt = FALSE
)
```

**Arguments**

intensity	intensity profile. See 'Details'.
intensity_str	structure of the intensity profile, options from ('SST_array', 'S_ST_mat', 'T_SS_mat'). See 'Details'.
pxsz	size of one pixel in unit of micron, 1 for simulated data
sz	frame size of the intensity profile in x and y directions, number of pixels contained in each frame equals sz_x by sz_y.
mindt	minimum lag time, 1 for simulated data
AIUQ_thr	threshold for wave number selection, numeric vector of two elements with values between 0 and 1. See 'Details'.
model_name	fitted model, options from ('BM', 'OU', 'FBM', 'OU+FBM', 'user_defined'), with Brownian motion as the default model. See 'Details'.
sigma_0_2_ini	initial value for background noise. If NA, use minimum value of absolute square of intensity profile in reciprocal space.
param_initial	initial values for param estimation.
num_optim	number of optimization.
msd_fn	user defined mean squared displacement(MSD) structure, a function of parameters and lag times. NA if model_name is not 'user_defined'.
msd_grad_fn	gradient for user defined mean squared displacement structure. If NA, then numerical gradient will be used for parameter estimation in 'user_defined' model.
num_param	number of parameters need to be estimated in the intermediate scattering function, need to be non-NA value for user_defined' model.
uncertainty	a logical evaluating to TRUE or FALSE indicating whether parameter uncertainty should be computed.
M	number of particles. See 'Details'.
sim_object	NA or an S4 object of class simulation.
msd_truth	true MSD or reference MSD value.
method	methods for parameter estimation, options from ('AIUQ', 'DDM_fixedAB', 'DDM_estAB').
index_q_AIUQ	index range for wave number when using AIUQ method. See 'Details'.
index_q_DDM	index range for wave number when using DDM method. See 'Details'.
message_out	a logical evaluating to TRUE or FALSE indicating whether or not to output the message.
A_neg	controls modification for negative A(q), options from ('abs', 'zero'), with setting negative A(q) to its absolute value as the default.
square	a logical evaluating to TRUE or FALSE indicating whether or not to crop the original intensity profile into square image.
output_dqt	a logical evaluating to TRUE or FALSE indicating whether or not to compute observed dynamic image structure function(Dqt).
output_isf	a logical evaluating to TRUE or FALSE indicating whether or not to compute empirical intermediate scattering function(ISF).

`output_modeled_isf`

a logical evaluating to TRUE or FALSE indicating whether or not to compute modeled intermediate scattering function(ISF).

`output_modeled_dqt`

a logical evaluating to TRUE or FALSE indicating whether or not to compute modeled dynamic image structure function(Dqt).

## Details

For simulated data using `simulation` in AIUQ package, intensity will be automatically extracted from `simulation` class.

By default `intensity_str` is set to 'T\_SS\_mat', a time by space×space matrix, which is the structure of intensity profile obtained from `simulation` class. For `intensity_str='SST_array'`, input intensity profile should be a space by space by time array, which is the structure from loading a tif file. For `intensity_str='S_ST_mat'`, input intensity profile should be a space by space×time matrix.

By default `AIUQ_thr` is set to `c(1, 1)`, uses information from all complete q rings. The first element affects maximum wave number selected, and second element controls minimum proportion of wave number selected. By setting 1 for the second element, if maximum wave number selected is less than the wave number length, then maximum wave number selected is coerced to use all wave number unless user defined another index range through `index_q_AIUQ`.

If `model_name` equals 'user\_defined', or NA (will coerced to 'user\_defined'), then `msd_fn` and `num_param` need to be provided for parameter estimation.

Number of particles `M` is set to 50 or automatically extracted from `simulation` class for simulated data using `simulation` in AIUQ package.

By default, using all wave vectors from complete q ring, unless user defined index range through `index_q_AIUQ` or `index_q_DDM`.

## Value

Returns an S4 object of class SAM.

## Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

## References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

**Examples**

```

library(AIUQ)
# Example 1: Estimation for simulated data
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)

```

---

SAM-class

*SAM class*


---

**Description**

S4 class for fast parameter estimation in scattering analysis of microscopy, using either AIUQ or DDM method.

**Slots**

`pxsz` numeric. Size of one pixel in unit of micron with default value 1.

`mindt` numeric. Minimum lag time with default value 1.

`sz` vector. Frame size of the intensity profile in x and y directions, number of pixels contained in each frame equals `sz_x` by `sz_y`.

`len_t` integer. Number of time steps.

`len_q` integer. Number of wave vector.

`q` vector. Wave vector in unit of  $\text{um}^{-1}$ .

`d_input` vector. Sequence of lag times.

`B_est_ini` numeric. Estimation of B. This parameter is determined by the noise in the system. See 'References'.

`A_est_ini` vector. Estimation of  $A(q)$ . Note this parameter is determined by the properties of the imaged material and imaging optics. See 'References'.

`I_o_q_2_ori` vector. Absolute square of Fourier transformed intensity profile, ensemble over time.

`q_ori_ring_loc_unique_index` list. List of location index of non-duplicate values for each q ring.

`model_name` character. Fitted model, options from ('BM','OU','FBM','OU+FBM','user\_defined').

`param_est` vector. Estimated parameters contained in MSD.

`sigma_2_0_est` numeric. Estimated variance of background noise.

`msd_est` vector. Estimated MSD.

`uncertainty` logical. A logical evaluating to TRUE or FALSE indicating whether parameter uncertainty should be computed.

`msd_lower` vector. Lower bound of 95% confidence interval of MSD.

`msd_upper` vector. Upper bound of 95% confidence interval of MSD.

msd\_truth vector. True MSD or reference MSD value.

sigma\_2\_0\_truth vector. True variance of background noise, non NA for simulated data using simulation.

param\_truth vector. True parameters used to construct MSD, non NA for simulated data using simulation.

index\_q vector. Selected index of wave vector.

Dqt matrix. Dynamic image structure function  $D(q, \Delta t)$ .

ISF matrix. Empirical intermediate scattering function  $f(q, \Delta t)$ .

I\_q matrix. Fourier transformed intensity profile with structure 'SS\_T\_mat'.

AIC numeric. Akaike information criterion score.

mle numeric. Maximum log likelihood value.

param\_uq\_range matrix. 95% confidence interval for estimated parameters.

modeled\_Dqt matrix. Modeled dynamic image structure function  $D(q, \Delta t)$ .

modeled\_ISF matrix. Modeled intermediate scattering function  $f(q, \Delta t)$ .

### Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

### References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

---

show.aniso_sam	<i>Show scattering analysis of microscopy for anisotropic processes (aniso_SAM) object</i>
----------------	--

---

### Description

Function to print the aniso\_SAM class object after the aniso\_SAM model has been constructed.

### Usage

```
show.aniso_sam(object)
```

### Arguments

object            an S4 object of class aniso\_SAM

**Value**

Show a list of important parameters in class aniso\_SAM.

**Author(s)**

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

**References**

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

**Examples**

```
library(AIUQ)

## Simulate BM and get estimated parameters using BM model
# Simulation
aniso_sim_bm = aniso_simulation(sz=100, len_t=100, sigma_bm=c(0.5, 0.3))
show(aniso_sim_bm)

# AIUQ method: fitting using BM model
aniso_sam = aniso_SAM(sim_object=aniso_sim_bm, AIUQ_thr=c(0.99, 0))
show(aniso_sam)
```

---

show.aniso\_simulation *Show anisotropic simulation object*

---

**Description**

Function to print the aniso\_simulation class object after the aniso\_simulation model has been constructed.

**Usage**

```
show.aniso_simulation(object)
```

**Arguments**

object            an S4 object of class aniso\_simulation

**Value**

Show a list of important parameters in class aniso\_simulation.

**Author(s)**

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

**References**

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

**Examples**

```
library(AIUQ)

# Simulate simple diffusion for 100 images with 100 by 100 pixels
aniso_sim_bm = aniso_simulation(sz=100, len_t=100, sigma_bm=c(0.5, 0.1))
show(aniso_sim_bm)
```

---

show.sam

*Show scattering analysis of microscopy (SAM) object*

---

**Description**

Function to print the SAM class object after the SAM model has been constructed.

**Usage**

```
show.sam(object)
```

**Arguments**

object            an S4 object of class SAM

**Value**

Show a list of important parameters in class SAM.

**Author(s)**

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

**References**

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

## Examples

```
library(AIUQ)

## Simulate BM and get estimated parameters using BM model
# Simulation
sim_bm = simulation(sz=100, len_t=100, sigma_bm=0.5)
show(sim_bm)

# AIUQ method: fitting using BM model
sam = SAM(sim_object=sim_bm)
show(sam)
```

---

show.simulation	<i>Show simulation object</i>
-----------------	-------------------------------

---

## Description

Function to print the simulation class object after the simulation model has been constructed.

## Usage

```
show.simulation(object)
```

## Arguments

object            an S4 object of class simulation

## Value

Show a list of important parameters in class simulation.

## Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

## References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

## Examples

```
library(AIUQ)

# Simulate simple diffusion for 100 images with 100 by 100 pixels
sim_bm = simulation(sz=100, len_t=100, sigma_bm=0.5)
show(sim_bm)
```

simulation

*Simulate 2D particle movement***Description**

Simulate 2D particle movement from a user selected stochastic process, and output intensity profiles.

**Usage**

```
simulation(
  sz = c(200, 200),
  len_t = 200,
  M = 50,
  model_name = "BM",
  noise = "gaussian",
  I0 = 20,
  Imax = 255,
  pos0 = matrix(NaN, nrow = M, ncol = 2),
  rho = 0.95,
  H = 0.3,
  sigma_p = 2,
  sigma_bm = 1,
  sigma_ou = 2,
  sigma_fbm = 2
)
```

**Arguments**

sz	frame size of simulated image with default <code>c(200, 200)</code> .
len_t	number of time steps with default 200.
M	number of particles with default 50.
model_name	stochastic process simulated, options from ('BM', 'OU', 'FBM', 'OU+FBM'), with default 'BM'.
noise	background noise, options from ('uniform', 'gaussian'), with default 'gaussian'.
I0	background intensity, value between 0 and 255, with default 20.
Imax	maximum intensity at the center of the particle, value between 0 and 255, with default 255.
pos0	initial position for M particles, matrix with dimension M by 2.
rho	correlation between successive step and previous step in O-U process, value between 0 and 1, with default 0.95.
H	Hurst parameter of fractional Brownian Motion, value between 0 and 1, with default 0.3.
sigma_p	radius of the spherical particle ( <code>3sigma_p</code> ), with default 2.

sigma_bm	distance moved per time step in Brownian Motion, with default 1.
sigma_ou	distance moved per time step in Ornstein–Uhlenbeck process, with default 2.
sigma_fbm	distance moved per time step in fractional Brownian Motion, with default 2.

**Value**

Returns an S4 object of class `simulation`.

**Author(s)**

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

**References**

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

**Examples**

```
library(AIUQ)
# -----
# Example 1: Simple diffusion for 200 images with
#           200 by 200 pixels and 50 particles
# -----
sim_bm = simulation()
show(sim_bm)

# -----
# Example 2: Simple diffusion for 100 images with
#           100 by 100 pixels and slower speed
# -----
sim_bm = simulation(sz=100, len_t=100, sigma_bm=0.5)
show(sim_bm)

# -----
# Example 3: Ornstein-Uhlenbeck process
# -----
sim_ou = simulation(model_name="OU")
show(sim_ou)
```

---

simulation-class      *Simulation class*

---

### Description

S4 class for 2D particle movement simulation.

### Details

`intensity` should have structure `'T_SS_mat'`, matrix with dimension `len_t` by `sz`×`sz`.

`pos` should be the position matrix with dimension `M`×`len_t`. See [bm\\_particle\\_intensity](#), [ou\\_particle\\_intensity](#), [fbm\\_particle\\_intensity](#), [fbm\\_ou\\_particle\\_intensity](#).

### Slots

`sz` vector. Frame size of the intensity profile, number of pixels contained in each frame equals `sz[1]` by `sz[2]`.

`len_t` integer. Number of time steps.

`noise` character. Background noise, options from (`'uniform'`, `'gaussian'`).

`model_name` character. Simulated stochastic process, options from (`'BM'`, `'OU'`, `'FBM'`, `'OU+FBM'`).

`M` integer. Number of particles.

`pxsz` numeric. Size of one pixel in unit of micron, 1 for simulated data.

`mindt` numeric. Minimum lag time, 1 for simulated data.

`pos` matrix. Position matrix for particle trajectory, see `'Details'`.

`intensity` matrix. Filled intensity profile, see `'Details'`.

`num_msd` vector. Numerical mean squared displacement (MSD).

`param` vector. Parameters for simulated stochastic process.

`theor_msd` vector. Theoretical MSD.

`sigma_2_0` vector. Variance of background noise.

### Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

### References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. *Physical Review E*, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. *Physical review letters*, 100(18), 188102.

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