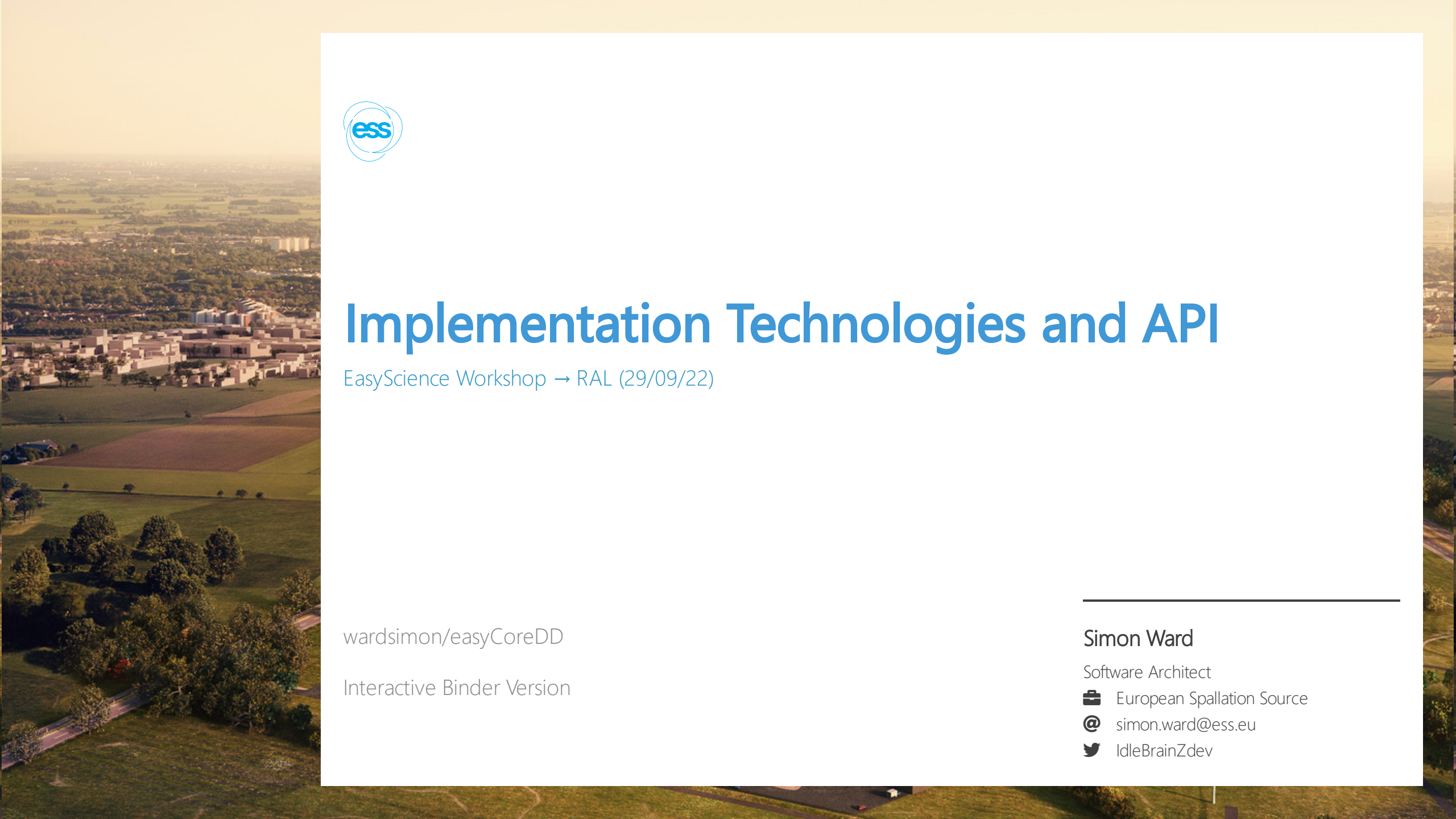

Implementation Technologies and API

EasyScience Workshop → RAL (29/09/22)

wardsimon/easyCoreDD

Interactive Binder Version

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Software Architect

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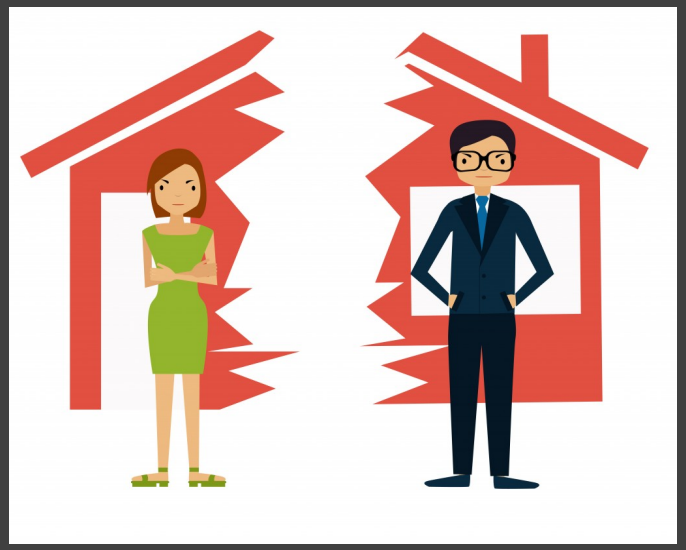
IdleBrainZdev

Presentation Outline

1. Separation of Assets, What is EasyCore
2. The features.
3. Code Examples.
4. Where are we going.

Separation of Assets, What is EasyCore



Ahluwalia-law.com

What are the aims.

1. Ability to create components from building blocks
2. Components can be optimized against data.
3. Optimization is **NOT** just LM
4. Components can offload calculations to established libraries.
5. Components can be reused.
6. Access to modern concepts made easy.

The building blocks.

Descriptors

- Named variables
- Not necessarily numbers
- Can not be used for optimization

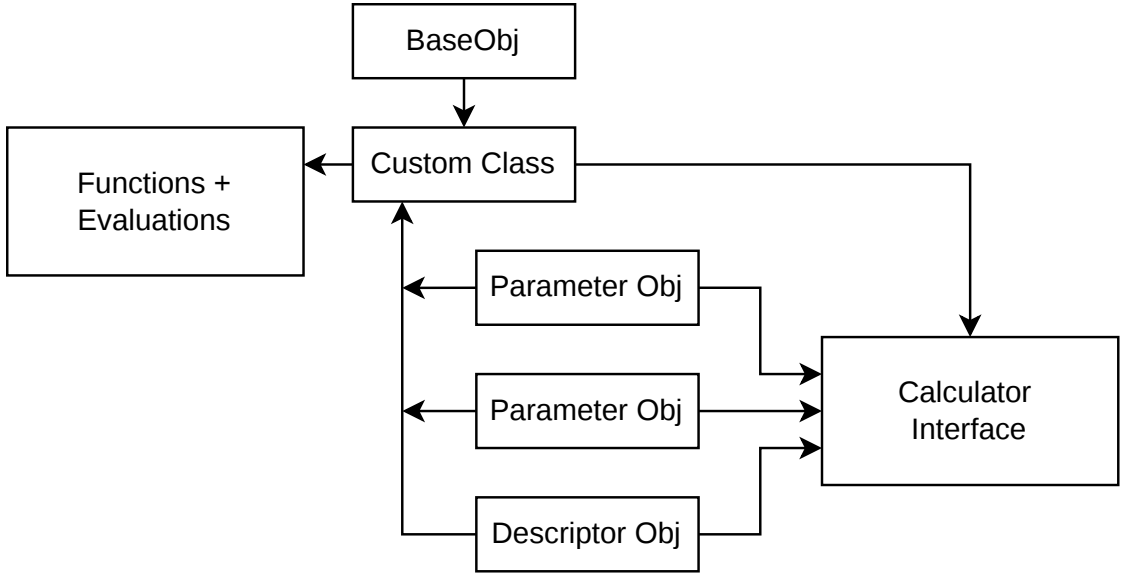
Parameters

- Based on Descriptors
- Only numbers
- Can be used for optimization

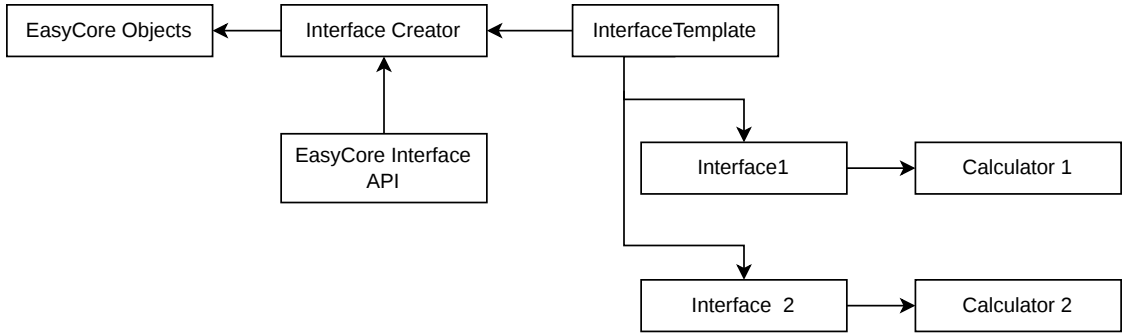
Base Objects

- Used to create components
- Can be composed of components and parameters
- Knows everything it's composed of
- Can be linked to an interface

Creating a Base Core Object



Creating an interface.



The Features

Ambreen Hasan, Unsplash license

Easy Interfacing

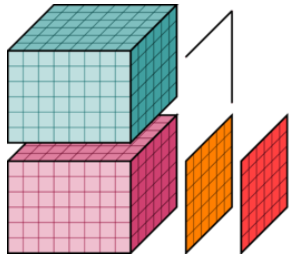
Shutterstock.

- Calculation not limited by a single backend
- Seamlessly switch
- No need to learn specific calculators

Easy Optimization

- LMfit, Bumps and DFO_LS libraries are available
- All methods of each libraries.
- Multi dimensional datasets.
- Multi objective optimization.
- Advanced constraints.
- Does not care about calculator

Easy Parallelization

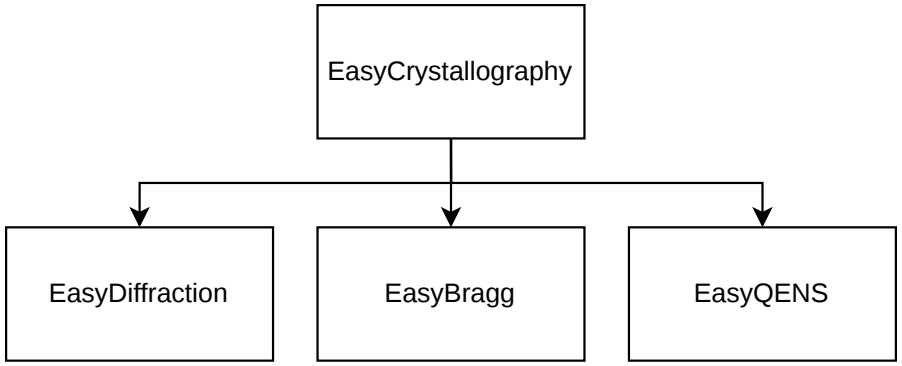


xarray

X-Array - Apache-2.0 license.

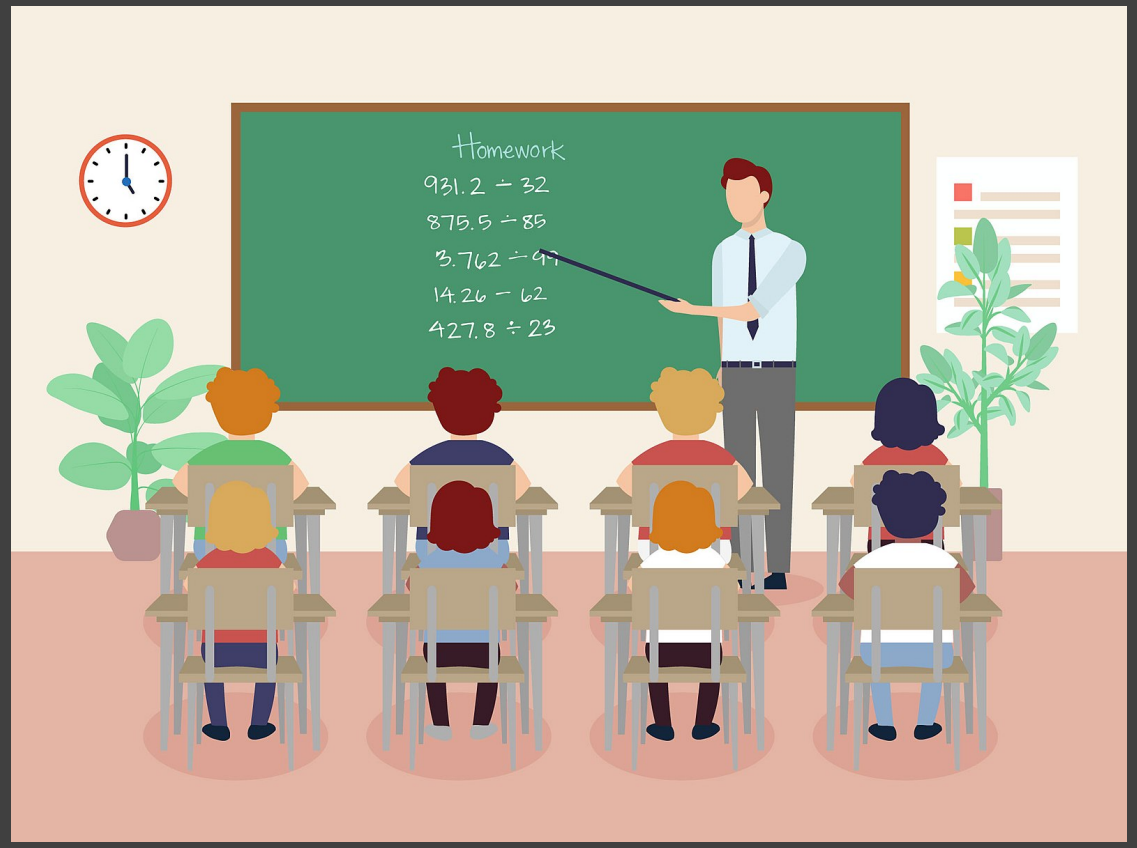
- Datasets can be stored in X-Array
- Dask scheduling built in
- Slicing and MPI

Reusable etc..



- Components are reusable across techniques
- Components can be dynamically added as needed
- Unit support and conversion.
- Json serialization and others supported.
- Undo/Redo support for all objects.
- Auto script generation (in development).

Lets get dirty...



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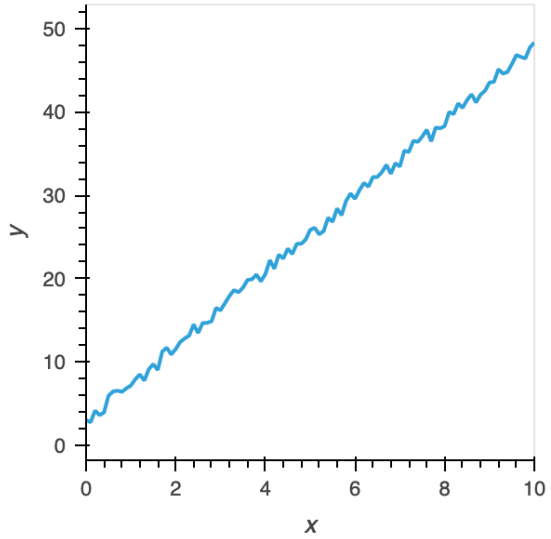
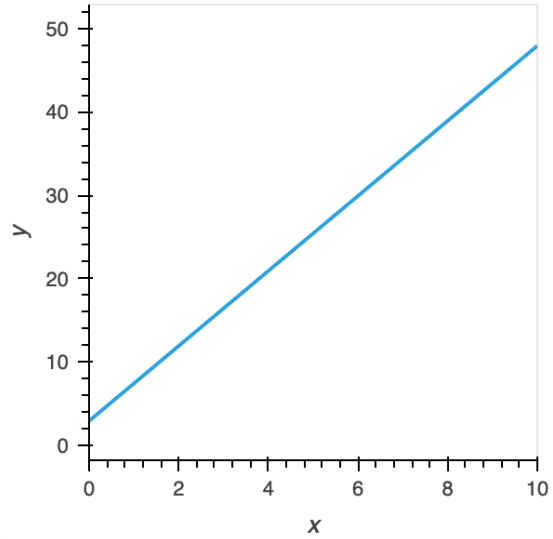
Example 1 - a Line :-/





- We show 2 methods for object creation
- We optimize values
- We use different minimizer libraries and methods

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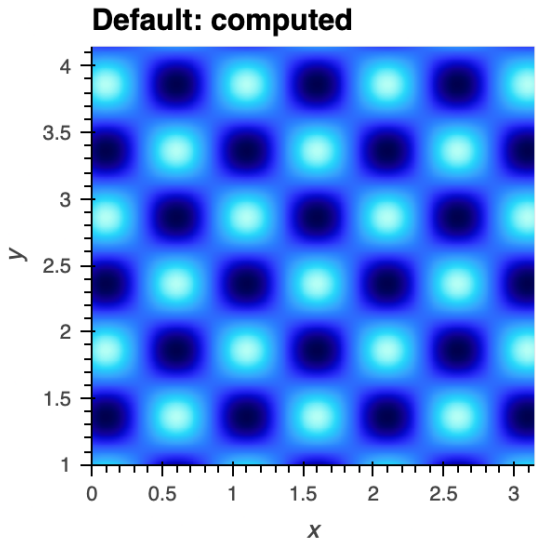
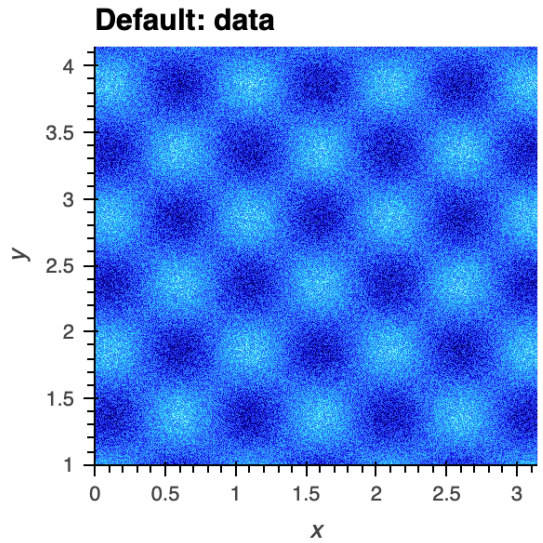
Example 2 - a 2D optimization





- We use x-array
- We optimize in 2D

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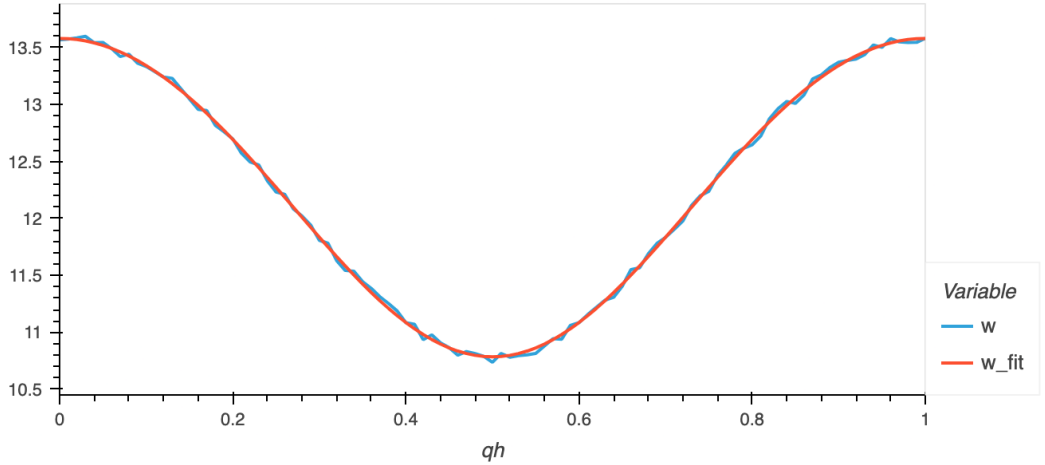
Example 3 - a real life example

A 4D optimization to a spin ladder model



- We use x-array
- We use ND visualization
- We optimize to a 4D dataset

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The future

brickshop.eu

Enhancing JuPyter Notebook support

- Use panel for better JuPyter integration
- Auto widgets
- Interactive web apps
- Leading to advanced callbacks

Work in progress…

JAX - Compilation, ML and Optimization

- Speed up calculations
- ND Convolutions
- ML applications?
- Custom autograd optimization

Available in an easyCore branch

PyMC3 - Bayesian optimization and modeling

- Use advanced Bayesian samplers
- Advanced optimization statistics
- Probability distributions, Gaussian process, Variational inference

Available in an easyCore branch