nrefocus Documentation

Release 0.4.0

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Nrefocus is a Python 3 library that allows to numerically refocus (including autofocusing) complex wave fields. This is the documentaion of nrefocus version 0.4.0.

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INTRODUCTION

This package provides methods for numerical propagation of a complex wave in free space. The available propagators are the angular spectrum method (*helmholtz*) and the Fresnel approximation (*fresnel*). Both implementations are convolution-based. The angular spectrum method is suited for near-field propagation (numerical focusing) and yields better results than the Fresnel approximation. The single Fourer transform-based Fresnel propagation method which is suitable for far-field propagation is not implemented in this package.

1.1 Obtaining nrefocus

You can install nrefocus via:

```
pip install nrefocus
```

If you would like to take advantage of fast Fourer transforms with PyFFTW, please also install the *pyfftw* package or use the extras key *FFTW*:

```
pip install nrefocus[FFTW]
```

The source code of nrefocus is available at https://github.com/RI-imaging/nrefocus.

1.2 Citing nrefocus

Please cite this package if you are using it in a scientific publication.

This package should be cited like this¹.

You can find out what version you are using by typing (in a Python console):

```
>>> import nrefocus
>>> nrefocus.__version__
'0.1.2'
```

¹ Paul Müller (2013) nrefocus: Python algorithms for numerical focusing (Version x.x.x) [Software]. Available at https://pypi.python.org/pypi/nrefocus/.

1.3 Acknowledgments

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1.4 References

THEORY

The derivations given here are treated in more detail in the relevant literature, e.g. [[ST91]] and [[Goo05]].

2.1 Optical transfer function

Let us consider a wave field $u(\mathbf{r_0})$ whose values we know at an initial plane $\mathbf{r_0} = (x_0, y_0, z_0)$ (z_0 fixed). The field has a certain vacuum wavelength λ and is traveling through a homogeneous medium with refractive index $n_{\rm m}$. From the knowledge of the wave field at the plane $\mathbf{r_0}$ and its wavelength $\lambda/n_{\rm m}$, we can infer the direction of propagation of the wave field for every point in $\mathbf{r_0}$. We rewrite the field at $\mathbf{r_0}$ as an angular spectrum, a sum over all possible directions $\mathbf{s} = (p, q, M)$, assuming that the field is only traveling from left to right

$$u(\mathbf{r_0}) = \iint dp dq \, A(p, q) e^{ik_{\rm m}(px_0 + qy_0 + Mz_0)}$$
$$|\mathbf{s}| = p^2 + q^2 + M^2 = 1$$
$$M = \sqrt{1 - p^2 - q^2}.$$

The equation above describes the Huygens-Fresnel principle: the value of the field u at a certain position $\mathbf{r_0}$ at the initial plane (point source) is defined as an integral over all possible plane waves with wavenumber $k_{\mathrm{m}} = \frac{2\pi n_{\mathrm{m}}}{\lambda}$, weighted with the amplitude A(p,q).

Let us now consider the 2D Fourier transform of $u(\mathbf{r_0})$.

$$\begin{split} \widehat{U}_{0}(k_{\mathbf{x}},k_{\mathbf{y}}) &= \frac{1}{2\pi} \iint \!\! dx_{0} dy_{0} \iint \!\! dp dq \, A(p,q) e^{ik_{\mathbf{m}}(px_{0}+qy_{0}+Mz_{0})} e^{-i(k_{\mathbf{x}}x_{0}+k_{\mathbf{y}}y_{0})} \\ &= \frac{1}{2\pi} \iint \!\! dx_{0} dy_{0} \iint \!\! dp dq \, A(p,q) e^{ik_{\mathbf{m}}Mz_{0}} e^{ix_{0}(k_{\mathbf{m}}p-k_{\mathbf{x}})} e^{iy_{0}(k_{\mathbf{m}}q-k_{\mathbf{y}})} \\ &= \frac{2\pi}{k_{\mathbf{m}}^{2}} A(k_{\mathbf{x}},k_{\mathbf{y}}) e^{ik_{\mathbf{m}}Mz_{0}} \end{split}$$

Here we made use of the identity of the delta distribution

$$\frac{1}{2\pi} \int dx_0 e^{ix_0(k_{\rm m}p - k_{\rm x})} = \delta(k_{\rm m}p - k_{\rm x}) = \frac{1}{k_{\rm m}} \delta(p - k_{\rm x}/k_{\rm m})$$
$$\frac{1}{2\pi} \int dy_0 e^{iy_0(k_{\rm m}q - k_{\rm y})} = \delta(k_{\rm m}q - k_{\rm y}) = \frac{1}{k_{\rm m}} \delta(q - k_{\rm y}/k_{\rm m})$$

If we now perform the same procedure for a different position $\mathbf{r}_{d} = (x_0, y_0, z_d)$, we will see that the Fourier transform of the field becomes

$$\widehat{U}_{\rm d}(k_{\rm x}, k_{\rm y}) = \frac{2\pi}{k_{\rm m}^2} A(k_{\rm x}, k_{\rm y}) e^{ik_{\rm m}Mz_{\rm d}}.$$

Thus, the propagation of the field $u(\mathbf{r_0})$ by a distance $d=z_{\rm d}-z_0$ is described by a multiplication with the transfer function

$$\mathcal{H}^{\text{Helmholtz}} = e^{ik_{\text{m}}Md}$$

in Fourier space. This is the basis of the convolution-based numerical propagation algorithms implemented in nrefocus. The process of numerical propagation with the angular spectrum method can be written as

$$u(\mathbf{r_d}) = \mathcal{F}^{-1} \{ \mathcal{F} \{ u(\mathbf{r_0}) \} \cdot e^{ik_{\text{m}}Md} \}$$

with the Fourier transform \mathcal{F} and its inverse \mathcal{F}^{-1} . With the convolution operator *, we may rewrite this equation to

$$u(\mathbf{r_d}) = u(\mathbf{r_0}) * \mathcal{F}^{-1} \left\{ e^{ik_{\rm m}Md} \right\}.$$

2.2 Fresnel approximation

The Fresnel approximation (or paraxial approximation) uses a Taylor expansion to simplify the exponent of the transfer function $e^{ik_{\rm m}Md}$. The exponent can be rewritten as

$$ik_{\rm m}Md = ik_{\rm m}d\left(1 - p^2 - q^2\right)^{1/2}$$
.

If the angles of propagation θ_x and θ_y for each plane wave of the angular spectrum is small, then we can make the paraxial approximation:

$$\theta_{x} \approx p$$

$$\theta_{y} \approx q$$

$$\theta^{2} = \theta_{x}^{2} + \theta_{y}^{2} \approx p^{2} + q^{2}$$

We now Taylor-expand the exponent around small values of θ

$$ik_{\rm m}d\left(1-\theta^2\right)^{1/2}\approx ik_{\rm m}d\left(1-\frac{\theta^2}{2}+\frac{\theta^4}{8}-\ldots\right).$$

The Fresnel approximation discards the third term ($\sim \theta^4$) and the transfer function then reads:

$$\begin{split} e^{ik_{\mathrm{m}}Md} &\approx e^{ik_{\mathrm{m}}d} \cdot e^{-\frac{ik_{\mathrm{m}}d(p^2+q^2)}{2}} \\ e^{i\sqrt{k_{\mathrm{m}}^2 - k_{\mathrm{x}}^2 - k_{\mathrm{y}}^2}d} &\approx e^{ik_{\mathrm{m}}d} \cdot e^{-\frac{id(k_{\mathrm{x}}^2 + k_{\mathrm{y}}^2)}{2k_{\mathrm{m}}}} \\ \mathcal{H}^{\mathrm{Fresnel}} &= e^{ik_{\mathrm{m}}d} \cdot e^{-\frac{id(k_{\mathrm{x}}^2 + k_{\mathrm{y}}^2)}{2k_{\mathrm{m}}}} \end{split}$$

Thus, the propagation by a distance distance $d=z_{\rm d}-d$ in the Fresnel approximation can be written in the form of the convolution

$$u(\mathbf{r_d}) = e^{ik_{\mathrm{m}}d} \cdot u(\mathbf{r_0}) * \mathcal{F}^{-1} \left\{ e^{-\frac{id(k_{\mathrm{x}}^2 + k_{\mathrm{y}}^2)}{2k_{\mathrm{m}}}} \right\}.$$

Note that the Fresnel approximation results in paraboloidal waves $(p^2 + q^2)$ whereas spherical waves are used with the Helmholtz equation.

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2.3 Transfer functions in nrefocus

The numerical focusing algorithms in this package require the input data $u_{\rm in}$ to be normalized by the incident plane wave $u_0({\bf r_0})$ according to

$$u_{\rm in}(\mathbf{r_0}) = \frac{u(\mathbf{r_0})}{u_0(\mathbf{r_0})}$$

As a result, the transfer functions change to

$$\begin{split} \mathcal{H}_{\text{norm}}^{\text{Helmholtz}} &= e^{ik_{\text{m}}(M-1)d} = e^{id\left(\sqrt{k_{\text{m}}^2 - k_{\text{x}}^2 - k_{\text{y}}^2} - k_{\text{m}}\right)} \\ \mathcal{H}_{\text{norm}}^{\text{Fresnel}} &= e^{-\frac{id(k_{\text{x}}^2 + k_{\text{y}}^2)}{2k_{\text{m}}}}. \end{split}$$

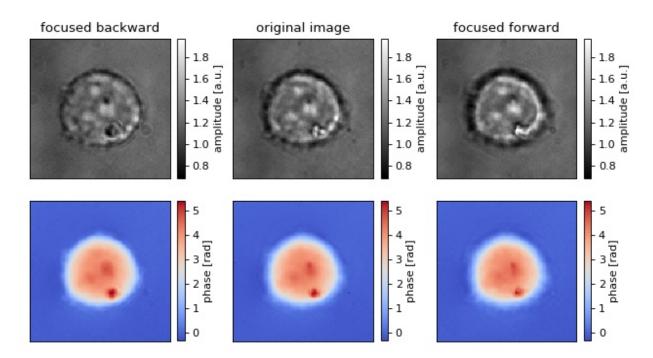
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EXAMPLES

3.1 2D Refocusing of an HL60 cell

The data show a live HL60 cell imaged with quadriwave lateral shearing interferometry (SID4Bio, Phasics S.A., France). The diameter of the cell is about $20\mu m$.



refocus_cell.py

```
import matplotlib.pylab as plt
import numpy as np
import unwrap

import nrefocus

from example_helper import load_cell

# load initial cell
cell1 = load_cell("HL60_field.zip")
```

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```
11
   # refocus to two different positions
12
   cell2 = nrefocus.refocus(cell1, 15, 1, 1) # forward
13
   cell3 = nrefocus.refocus(cell1, -15, 1, 1) # backward
14
15
   # amplitude range
16
   vmina = np.min(np.abs(cell1))
17
   vmaxa = np.max(np.abs(cell1))
18
   ampkw = {"cmap": plt.get_cmap("gray"),
19
             "vmin": vmina,
20
             "vmax": vmaxa}
21
   # phase range
   cell1p = unwrap.unwrap(np.angle(cell1))
24
   cell2p = unwrap.unwrap(np.angle(cell2))
25
   cell3p = unwrap.unwrap(np.angle(cell3))
26
   vminp = np.min(cell1p)
27
   vmaxp = np.max(cell1p)
   phakw = {"cmap": plt.get_cmap("coolwarm"),
29
             "vmin": vminp,
30
             "vmax": vmaxp}
31
32
   # plots
33
   fig, axes = plt.subplots(2, 3, figsize=(8, 4.5))
34
   axes = axes.flatten()
   for ax in axes:
37
       ax.xaxis.set_major_locator(plt.NullLocator())
       ax.yaxis.set_major_locator(plt.NullLocator())
38
39
   # titles
40
   axes[0].set_title("focused backward")
41
   axes[1].set_title("original image")
   axes[2].set_title("focused forward")
43
44
   # data
45
   mapamp = axes[0].imshow(np.abs(cell3), **ampkw)
46
47
   axes[1].imshow(np.abs(cell1), **ampkw)
   axes[2].imshow(np.abs(cell2), **ampkw)
   mappha = axes[3].imshow(cell3p, **phakw)
   axes[4].imshow(cell1p, **phakw)
50
   axes[5].imshow(cell2p, **phakw)
51
52
   # colobars
53
   cbkwargs = {"fraction": 0.045}
54
   plt.colorbar(mapamp, ax=axes[0], label="amplitude [a.u.]", **cbkwargs)
   plt.colorbar(mapamp, ax=axes[1], label="amplitude [a.u.]", **cbkwargs)
   plt.colorbar(mapamp, ax=axes[2], label="amplitude [a.u.]", **cbkwargs)
57
   plt.colorbar(mappha, ax=axes[3], label="phase [rad]", **cbkwargs)
   plt.colorbar(mappha, ax=axes[4], label="phase [rad]", **cbkwargs)
60
   plt.colorbar(mappha, ax=axes[5], label="phase [rad]", **cbkwargs)
   plt.tight_layout()
   plt.show()
```

FOUR

CODE REFERENCE

4.1 Refocus interface

Refocus is a user-convenient interface for numerical refocusing. Each class implements refocusing for a specific dimensionality (1D or 2D fields) using a specific method for refocusing (e.g. numpy FFT or FFTW).

4.2 Metrics

4.3 Legacy methods

These methods are legacy functions which are kept for backwards-compatibility.

4.3.1 Refocusing

4.3.2 Autofocusing

CHANGELOG

List of changes in-between nrefocus releases.

5.1 version 0.4.0

- feat: implement nrefocus.RefocusPyFFTW for faster refocusing using pyfftw
- enh: speed-up propagation kernel computation using numexpr
- · docs: cleanup

5.2 version 0.3.1

• dist: include submodules in wheel/dist

5.3 version 0.3.0

- feat: introduce nrefocus.RefocusNumpy and nrefocus.RefocusNumpy1D interface class for user-convenience and efficiency
- · docs: cleanup
- ref: new submodule for metrics and metrics now accept a Refocus instance as an argument
- · ref: new submodule for minimizers and minimizers now accept a Refocus instance
- ref: make legacy autofocusing code use the new Refocus class

5.4 version 0.2.1

- fix: fix several minor bugs (deprecations?) that caused the tests to faile
- ci: migrate to GitHub Actions
- setup: setup.py test is deprecated
- docs: refurbish documentation

5.5 version 0.2.0

- Drop support for Python 2 (#8)
- Code cleanup

5.6 version 0.1.8

• Include docs in sdist

5.7 version 0.1.7

• Update documentation and examples

5.8 version 0.1.6

- Move documentation from GitHub to readthedocs.io
- · Add universal wheel on PyPI
- Update tests on travis with new versions of NumPy

5.9 version 0.1.5

· Code cleanup

5.10 version 0.1.4

- Padding is now available in all methods (#2)
- Added new convenient submodule pad
- Bugfix: autofocusing did not return the correct focusing distance. This resulted in a slight offset in the refocusing distance for the method *autofocus_stack* when *same_dist=True* was set.
- New test functions for pad

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BILBLIOGRAPHY

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INDICES AND TABLES

- genindex
- modindex
- search

BIBLIOGRAPHY

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