Polsim

A case study for scientific computing in Rust

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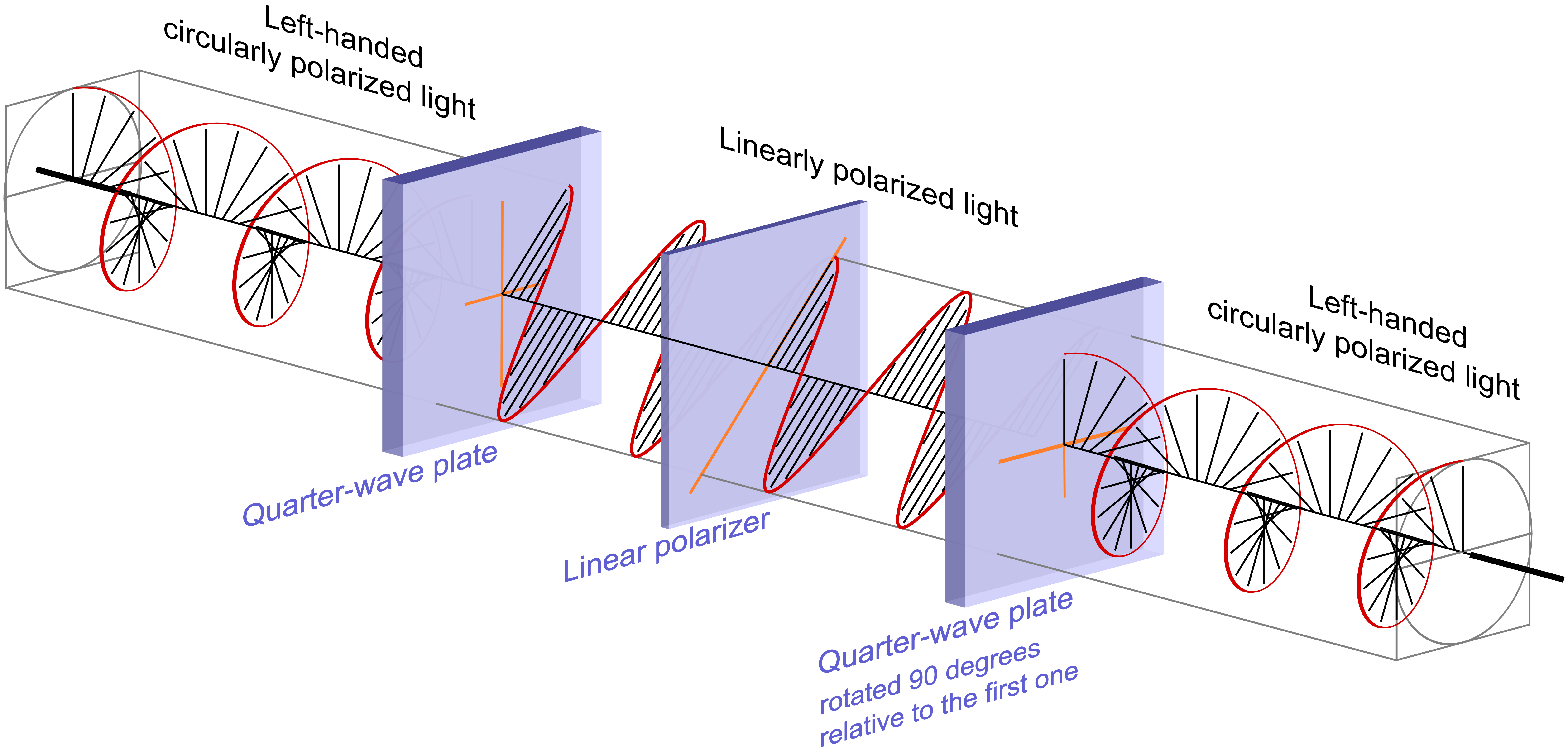
polsim

CLI tool for *pol*arization *sim*ulations

Project structure

- `polarization`
  - Crate I wrote for the polarization simulations
  - Uses a technique called Jones calculus
- `polsim`
  - Provides a CLI for `polarization`


Left-handed
circularly polarized light
Linearly polarized light
Left-handed
circularly polarized light
Quarter-wave plate
Linear polarizer
Quarter-wave plate
rotated 90 degrees
relative to the first one

Jones calculus primer

Polarization is a vector with two components:

$$\vec{E} = \begin{bmatrix} A \\ Be^{i\delta} \end{bmatrix} = \begin{bmatrix} \text{complex number} \\ \text{complex number} \end{bmatrix}$$

Optical elements that interact with the beam are 2x2 matrices:

$$M = \begin{bmatrix} m_{00} & m_{01} \\ m_{10} & m_{11} \end{bmatrix} = \begin{bmatrix} \text{complex} & \text{complex} \\ \text{complex} & \text{complex} \end{bmatrix}$$

Jones calculus primer

Multiply initial polarization by the optical elements to get the final polarization

$$E_f = M_N \times \ldots \times M_2 \times M_1 \times E_i$$

When you get down to it, you're just multiplying 2x2 matrices.

Those matrices can be pretty ugly…

$$\begin{bmatrix} \cos^2(\theta) + e^{i\varphi}\sin^2(\theta) & \sin(\theta)\cos(\theta) - e^{i\varphi}\sin(\theta)\cos(\theta) \\ \sin(\theta)\cos(\theta) - e^{i\varphi}\sin(\theta)\cos(\theta) & \sin^2(\theta) + e^{i\varphi}\cos^2(\theta) \end{bmatrix}$$

No one has ever used this matrix without looking it up

Translation to Rust

- Complex numbers
  - `num::complex::Complex<T>`
- Vectors
  - `nalgebra::Vector2<T>`
- Matrices
  - `nalgebra::Matrix2<T>`

Struggle #1 – debugging

```
(lldb) br set -f system.rs -l 348
Breakpoint 1: where = polarization-b20b1f754e235950`polarization
::jones::system::OpticalSystem::composed_elements
::_$u7b$$u7b$closure$u7d$$u7d$
::h19d2e65336af7615 + 577 at system.rs:348:30, address = 0x00000001001e8c11
```

Struggle #2 – debugging nalgebra

```
Process 33329 stopped
* thread #2, name = 'jones::system::test::test_beam_passes_through', stop reason = breakpoint 1.1
    frame #0: 0x000000001001e8c11 polarization-b20b1f754e235950`polarization::jones::system::OpticalSystem
    ::composed_elements::_$u7b$$u7b$closure$u7d$$u7d$::h19d2e65336af7615((null)=0x000070000ef72f98,
    acc=Matrix<num_complex::Complex<f64>, nalgebra::base::dimension::U2, nalgebra::base::dimension::U2,
    nalgebra::base::matrix_array::MatrixArray<num_complex::Complex<f64>, nalgebra::base::dimension::U2,
    nalgebra::base::dimension::U2>> @ 0x000070000ef73030, elem=0x0000000100c16aa0) at system.rs:348:30
```

Half of this debug message is just about the type of the matrix!

Struggle #2 - debugging nalgebra

```
(lldb) fr v
(closure *)  = 0x000070000ef72f98
(nalgebra::base::matrix::Matrix<num_complex::Complex<double>, nalgebra::base::dimension::U2,
nalgebra::base::dimension::U2, nalgebra::base::matrix_array::MatrixArray<num_complex::Complex<double>,
nalgebra::base::dimension::U2, nalgebra::base::dimension::U2> >) acc = {
  data = {
    data = {
      data = {
        parent1 = {
          parent1 = {
            parent1 = <Unable to determine byte size.>

            parent2 = <Unable to determine byte size.>

            data = (re = 1, im = 0)
          }
          parent2 = {
            parent1 = <Unable to determine byte size.>

            parent2 = <Unable to determine byte size.>

            data = (re = 0, im = 0)
          }
          _marker = {}
        }
        parent2 = {
          parent1 = {
            parent1 = <Unable to determine byte size.>

            parent2 = <Unable to determine byte size.>

            data = (re = 0, im = 0)
          }
          parent2 = {
            parent1 = <Unable to determine byte size.>

            parent2 = <Unable to determine byte size.>

            data = (re = 1, im = 0)
          }
          _marker = {}
        }
        _marker = {}
      }
    }
  }
  _phantoms = {}
}
(polarization::jones::system::OpticalElement *) elem = 0x0000000100c16aa0
(nalgebra::base::matrix::Matrix<num_complex::Complex<double>, nalgebra::base::dimension::U2,
nalgebra::base::dimension::U2, nalgebra::base::matrix_array::MatrixArray<num_complex::Complex<double>,
nalgebra::base::dimension::U2, nalgebra::base::dimension::U2> >) mat = {
  data = {
    data = {
      data = {
        parent1 = {
          parent1 = {
            parent1 = <Unable to determine byte size.>

            parent2 = <Unable to determine byte size.>

            data = (re = 1, im = 0)
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          parent2 = {
            parent1 = <Unable to determine byte size.>

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            parent2 = <Unable to determine byte size.>

            data = (re = 1, im = 0)
          }
          _marker = {}
        }
        _marker = {}
      }
    }
  }
  _phantoms = {}
}
```

Zoom

Struggle #2 – debugging nalgebra

```
(nalgebra::base::matrix::Matrix<num_complex::Complex<double>, nalgebra::base::dimension::U2,
nalgebra::base::dimension::U2, nalgebra::base::matrix_array::MatrixArray<num_complex::Complex<double>,
nalgebra::base::dimension::U2, nalgebra::base::dimension::U2> >) mat = {
  data = {
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          parent2 = {
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            parent2 = <Unable to determine byte size.>

            data = (re = 0, im = 0)
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          _marker = {}
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            parent1 = <Unable to determine byte size.>

            parent2 = <Unable to determine byte size.>

            data = (re = 1, im = 0)
          }
          _marker = {}
        }
        _marker = {}
      }
    }
  }
  _phantoms = {}
}
```

Enhance!

Struggle #2 – debugging nalgebra

The elements of a 2x2 matrix…

```
...
data = (re = 1, im = 0)
...
data = (re = 0, im = 0)
...
data = (re = 0, im = 0)
...
data = (re = 1, im = 0)
...
```

Information density is very low in debug output

JonesVector trait

```rust
pub trait JonesVector {
    // Intensity of the beam
    fn intensity(&self) -> Result<f64>;

    // Returns the x-component of the beam
    fn x(&self) -> f64;

    // Returns the y-component of the beam
    fn y(&self) -> f64;

    ...
}
```

Beam

```rust
// Basically a container for the Vector2<T>
pub struct Beam {
    vec: Vector2<Complex<f64>>,
}

impl JonesVector for Beam {
    ...
}
```

JonesMatrix trait

Represents an optical element

```rust
pub trait JonesMatrix {
    // Rotate the element by the given angle
    fn rotated(&self, angle: Angle) -> Self;

    // Return the inner matrix of the element
    fn matrix(&self) -> Matrix2<Complex<f64>>;

    ...
}
```

Optical elements

Optical elements implement `JonesMatrix`

```rust
// An ideal linear polarizer
pub struct Polarizer {
    mat: Matrix2<Complex<f64>>,
}

impl JonesMatrix for Polarizer {
    ...
}
```

Putting it all together

```
let beam = ...
let e1 = ...
let e2 = ...
let system = OpticalSystem::new()
    .add_beam(beam)
    .add_element(e1)
    .add_element(e2);
let final_beam = system.propagate().unwrap();
```

Testing

- This is science
- Results should be:
  - reproducible
  - correct
  - etc

Science

❤

Property Based Testing

Property based testing (PBT)

- Unit tests
  - "The sum of 2 and 2 should be 4."
- Property based tests
  - "The sum of positive integers **x** and **y** should be positive."
  - **x** and **y** are typically randomly generated
  - The test is run with many randomly generated inputs

PBT and polarization

Tons of opportunities for soundness checks
- "No beam can pass through two crossed polarizers."
- "A beam that's rotated 360 degrees should look the same."
- "An optical element that's rotated 360 degrees should look the same."
- etc.

PBT in Rust – proptest

Generate arbitrary instances of your types

```rust
// Arbitrary trait from proptest
impl Arbitrary for Angle {
    type Parameters = ();
    type Strategy = BoxedStrategy<Self>;

    fn arbitrary_with(_: Self::Parameters) -> Self::Strategy {
        prop_oneof![
            (any::<f64>()).prop_map(|x| Angle::Degrees(x)),
            (any::<f64>()).prop_map(|x| Angle::Radians(x)),
        ]
        .boxed()
    }
}
```

PBT in Rust – proptest

Compose arbitrary instances from other arbitrary instances

```
impl Arbitrary for Polarizer {
    type Parameters = ();
    type Strategy = BoxedStrategy<Self>;

    fn arbitrary_with(_: Self::Parameters) -> Self::Strategy {
        any::<Angle>()  // select an arbitrary angle
            .prop_map(|angle| Polarizer::new(angle))  // use it to make a polarizer
            .boxed()
    }
}
```

Struggle #3 – floating point numbers

This happened several times:
– Test fails

Struggle #3 – floating point numbers

This happened several times:
- Test fails
- Debug the code

Struggle #3 – floating point numbers

This happened several times:
- Test fails
- Debug the code
- Realize the test is broken

Struggle #3 – floating point numbers

```
let x = ...; // randomly generated
loop {
    if x > pi / 2.0 {
        x -= pi;
        continue;
    } else if x < -pi / 2.0 {
        x += pi;
        continue;
    }
    break;
}
```

Hangs because `x = 5.1e+164` and `5.1e+164 + pi = 5.1e+164`

polsim

High level overview

- The user writes a simulation definition file.
- The file is read into a struct using `serde`.
- The simulation definition is validated.
- The simulation is performed.
- The results are printed.

Simulation definition

```
[beam]
polarization = "linear"
angle = 90
angle_units = "degrees"

[[elements]]
element_type = "polarizer"
angle = 45
angle_units = "degrees"

[[elements]]
element_type = "qwp"
angle = 0
angle_units = "degrees"
```

Beam definition

```rust
#[derive(Debug, Deserialize, Serialize)]
pub struct BeamDef {
    pub polarization: PolType,
    pub angle: Option<f64>,
    pub angle_units: Option<AngleType>,
    pub x_mag: Option<f64>,
    pub x_phase: Option<f64>,
    pub y_mag: Option<f64>,
    pub y_phase: Option<f64>,
    pub phase_units: Option<AngleType>,
    pub handedness: Option<HandednessType>,
}
```

Validation

```
fn validate_element(elem: &ElemDef) -> Result<OpticalElement> {
    match elem.element_type {
        ElemType::Polarizer => {
            validate_polarizer(elem).chain_err(|| "invalid polarizer definition")
        }
        ElemType::HWP => validate_hwp(elem).chain_err(|| "invalid half-wave plate definition"),
        ElemType::QWP => validate_qwp(elem).chain_err(|| "invalid quarter-wave plate definition"),
        ElemType::Retarder => validate_retarder(elem).chain_err(|| "invalid retarder definition"),
        ElemType::Rotator => {
            validate_rotator(elem).chain_err(|| "invalid polarization rotator definition")
        }
    }
}
```

Validation

```rust
fn validate_polarizer(elem: &ElemDef) -> Result<OpticalElement> {
    if elem.element_type != ElemType::Polarizer {
        return Err(ErrorKind::WrongElementType(format!(
            "Expected to validate element type Polarizer, found {:#?} instead",
            elem.element_type
        ))
        .into());
    }
    error_on_extra_params!(elem, phase, phase_units);
    let angle_res =
        validate_angle(&elem.angle, &elem.angle_units).chain_err(|| "invalid angle definition");
    match angle_res {
        Err(err) => Err(err),
        Ok(angle) => Ok(OpticalElement::Polarizer(Polarizer::new(angle))),
    }
}
```

Errors

Using `error-chain` to provide breadcrumbs for the user.

```
$ polsim has_error.toml
error: invalid system definition
caused by: invalid element definition
caused by: invalid polarizer definition
caused by: invalid angle definition
caused by: missing parameter in definition: 'angle_units'
```

Output

Pretty basic at the moment:

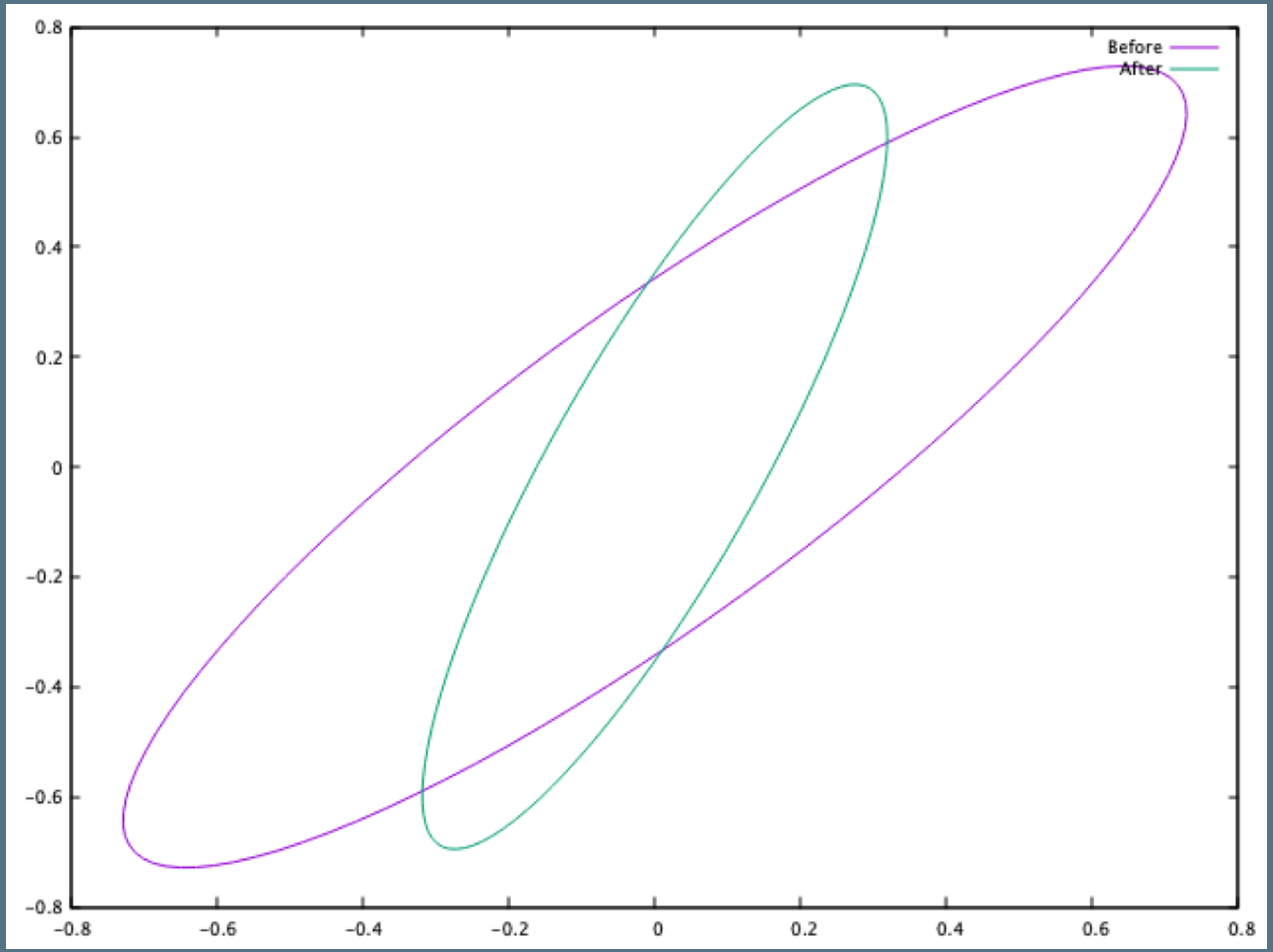
```
$ polsim examples/circular_polarizer.toml
intensity: 5.00000e-1
x_mag: 5.00000e-1
x_phase: 0.00000e0
y_mag: 5.00000e-1
y_phase: 1.57080e0
```

or

```
$ polsim --table examples/circular_polarizer.toml
+-----------+-----------+----------+-----------+----------+
| intensity | x_mag     | x_phase  | y_mag     | y_phase  |
+-----------+-----------+----------+-----------+----------+
| 5.00000e-1 | 5.00000e-1 | 0.00000e0 | 5.00000e-1 | 1.57080e0 |
+-----------+-----------+----------+-----------+----------+
```

Next steps

- Gnuplot output
- Missing optical elements (reflections)
- Rust 2018
- Parameter sweeps



Contact

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