

# Intro to Coding Best Practices for Shared Projects

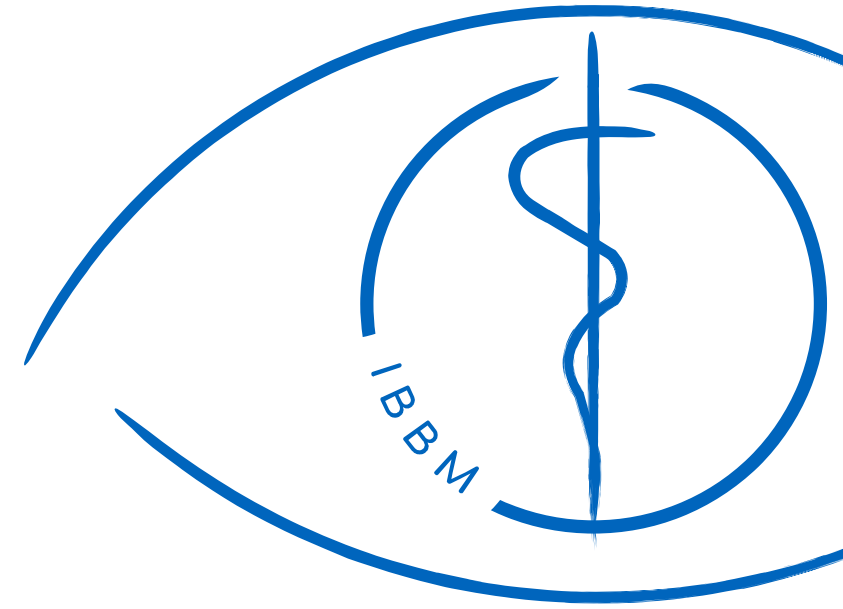
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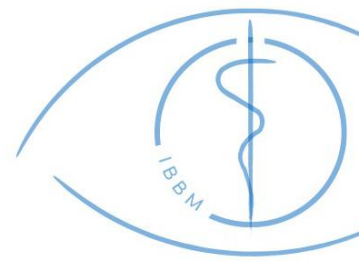
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Technical University of Munich

MRS Hackathon, Toronto

June 02, 2023





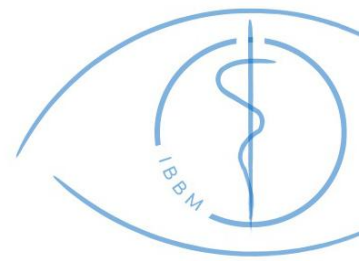
# Focus

## Coding *best practices* for shared projects

- Collaborations
- Theses
- Projects to be handed over to someone else

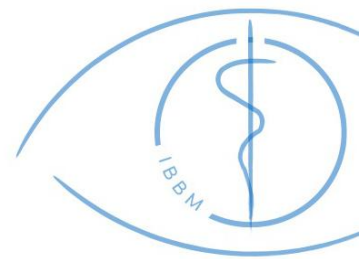


<https://www.apm.org.uk/v2/media/vjufacmf/shutterstock603988838.jpg>



# Coding

- Anyone can write working code. Making it work is easy.
- Most people write “*working code*”, not “*good code*”
- *Good code* should be:
  - **Organized**
  - Reliable
  - **Maintainable**
  - Efficient
  - **Documented**



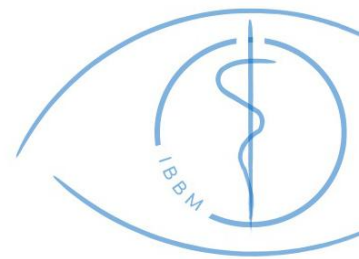
# Organized

## Getting Started with Big Projects

### Plan ahead!

- Objectives
- Functionality
- Requirements
- Completion checklist
- What will happen with the code?





# Example: Data Simulator

## Starting Point

### Goal:

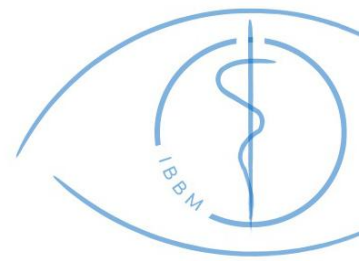
1. Robust physics model
2. Include everything possible

“I’ll figure it out as I go...”

## Better Developed

### Goal:

1. Maximize the degrees of freedom
2. Include all clinically relevant artifacts
  - List them out
3. Simulations should match specific use case(s)
  - What does this mean specifically?
4. Framework and compute requirements?
5. Community-driven development

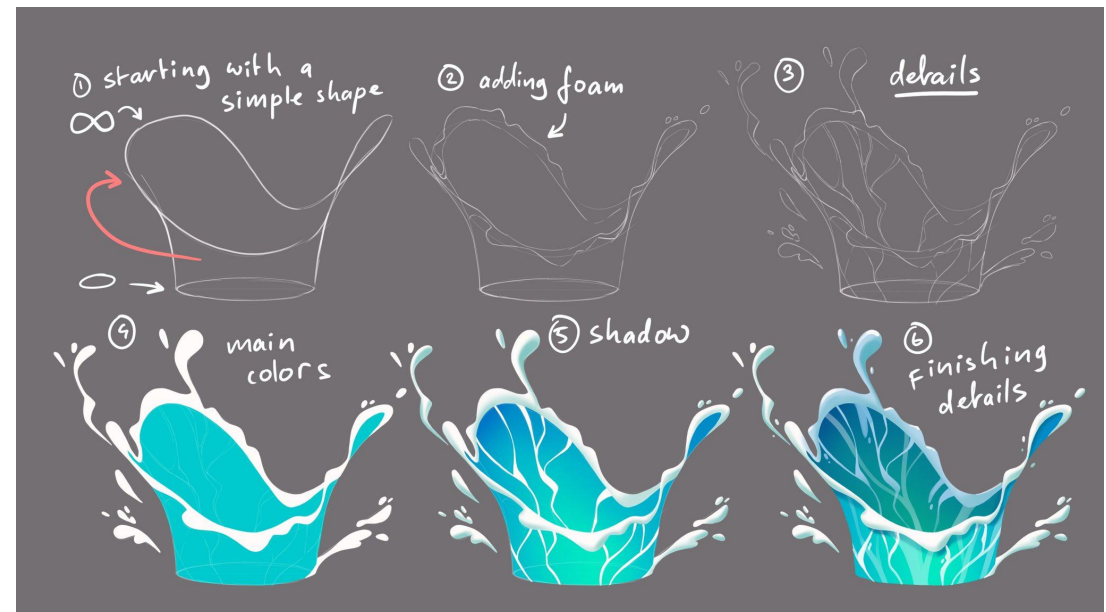


# Organized

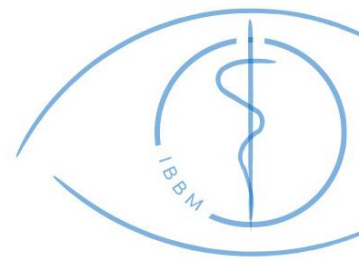
## Hierarchy of complexity!

### Always start simple!

- Start with the basics
- Iteratively debug
- Add more complexity and repeat



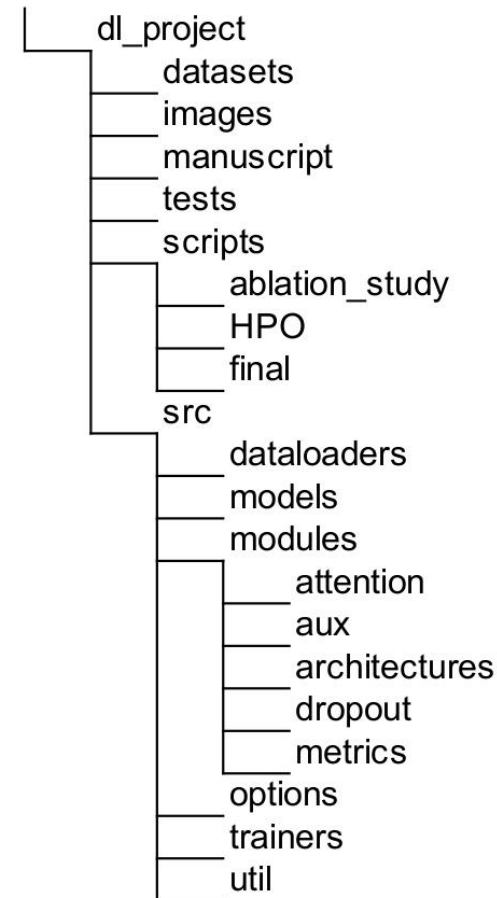
[https://pbs.twimg.com/media/FtRQeq\\_XoAAz7b6.jpg:large](https://pbs.twimg.com/media/FtRQeq_XoAAz7b6.jpg:large)

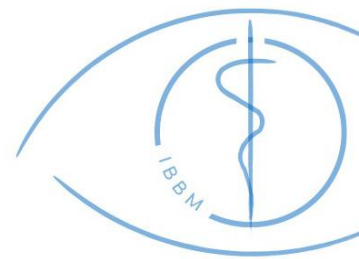


# Organized

## Tips for staying organized...

- Layout your project
  - A good layout should work for multiple (similar) projects
- Use the folders!
  - Save things where they belong
- Use version control to track and update your changes
  - Very useful for when you break something!
- Save experiment descriptions
  - E.g. ablation\_exp\_001\_config.json





# Reliability

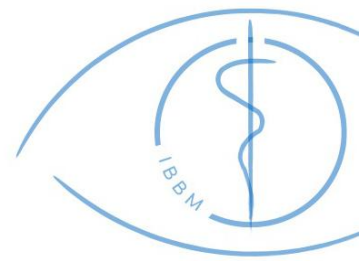
***“the quality of being trustworthy or of performing consistently well.”***

**- Oxford Dictionary**

**What does this look like in practice? — *Defensive programming***

- Assert statements and unit tests
  - Validate inputs
  - Boundary checks
- Error handling
- When are they necessary?





# Reliability

## *Example: Fourier Transform*

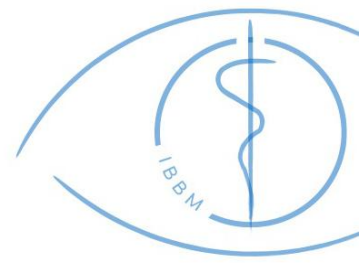
### Expectations:

- Input is at least a 3D matrix
  - n-dimensional tensor of 1D data
- The last dimension needs size=2
  - input data type is complex
  - Typical inputs should need to be transposed to satisfy this condition
- `torch.view_as_complex` expects contiguous inputs
- Separate outputs' real and imaginary in second to last dimension
- Output should be contiguous

### Expected input:

`signal.shape = [batchSize, ..., channels=2, spectral_length]`

```
def Fourier_Transform(signal: torch.Tensor) -> torch.Tensor:
    assert(signal.ndim>=3)
    if signal.shape[-2]==2:
        signal = signal.transpose(-1,-2)
    assert(signal.shape[-1]==2)
    signal = torch.view_as_complex(signal.contiguous())
    signal = torch.view_as_real(fftshift(fft(signal, dim=-1),
                                         dim=-1)).transpose(-1,-2)
    return signal.contiguous()
```

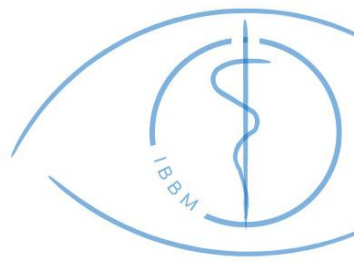


# Maintainability

***The ability to update and improve a code base and to fix problems when they arise.***

To maintain code, one needs to be able to:

- Read the code,
- Understand the code, and
- Fix the code.

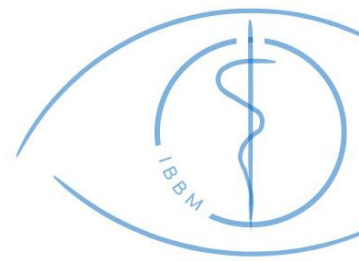


# Maintainability

***“Readability improves understanding; that further improves maintainability”***

-Cynthia Nelson

**Scenario:** 10 colleagues each use their own coding conventions. How does that affect code readability and maintainability?



# Maintainability

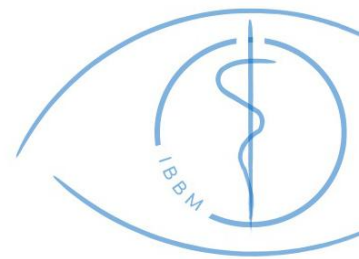
## Coding conventions

*For your own projects,*

- **Always be consistent**
- Follow the conventions for your selected framework

*For collaborations,*

- Define (non-standard) conventions at the beginning
- **Always be consistent**
- Limit exceptions



# Maintainability

## Naming conventions

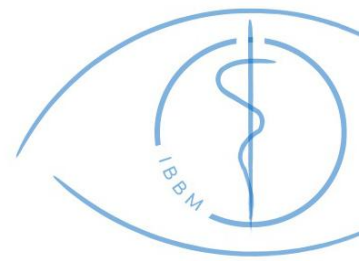
- **Camel case**
  - Ex. `firstName` and `lastName`
- **Snake case**
  - Ex. `first_name` and `last_name`
- **Kebab case**
  - Ex. `first-name` and `last-name`
- **Pascal case**
  - Ex. `FirstName` and `LastName`

## Python:

- variable & function names use Snake case
- classes use Pascal case

## JavaScript:

- variable & function names use Camel case
- classes use Pascal case



# Maintainability

## Formatting conventions

### Spacing

```
names = ['d',      'dmm', 'g',      'gmm']
mult  = [ 1, self.MM,  1, self.MM]
```

---

```
dB0  = x * x.transpose(-3,-2) / dx
dB0 += y
dB0  = dB0 + z
dB0 += mean
```

### Temporary variables

- for **i** in range(x): vs for **n** in range(x):
- for **key**, **value** in dct.items() vs  
for **k**, **v** in dct.items():

### File and function names

Be consistent with existing code!

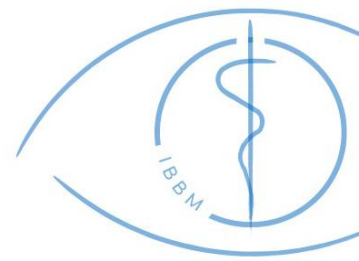
Consistency through out a project  
looks more professional

Quasi-exception: *nesting*

- Should still be consistent!

Nested for-loops: Avoid using **x** and **y**!

- for **i** in range(data.shape[1]):  
for **ii** in range(data.shape[2]):
- Example pairs: **i**, **ii** vs **j**, **k** vs **i**, **n** vs **n**, **m**



# Maintainability

## Modularity and Reusability

- In-line coding vs Modular Programming

```
p = params[:,self.index['metabolites']].unsqueeze(-1).unsqueeze(-1)
fid = p.repeat_interleave(2, dim=-2).mul(self.syn_basis_fids)

# Define basis spectra coefficients
if gen: print('>>>> Preparing metabolite coefficients')
fid = self.modulate(fids=self.syn_basis_fids,
                    params=params[:,self.index['metabolites']])
```

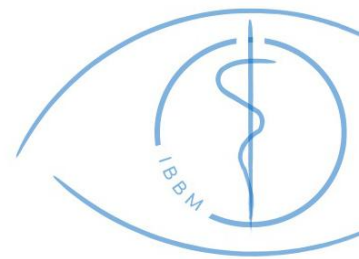
Function calls in my simulator

- 35 regular functions (inside the simulator class),
- 22 auxiliary functions (outside the simulator class), and
- 3 primary functions for running the simulations.
  - Currently >2400 lines of code in modular format

## Benefits of Modular Programming:

- Fewer lines of code
- Easier to read
- Easier to maintain
- Easier to debug
- Easier to document
- Defensive programming!





# Maintainability

## In-line/Modular Mix

```
# Add Noise
if noise:
    if gen: print('>>>>> Adding noise')
    transients, zeros = None, None
    if multicoil>1:
        transients = params[:,self.index['coil_snr']]
        zeros = torch.where(params[:,self.index['coil_sens']]<=0.0,
                             1,0).sum(dim=-1,keepdims=True)
    noise = self.generate_noise(fid=fidSum,
                                max_val=mx_values,
                                param=params[:,self.index['snr']],
                                zeros=zeros, # num of zeroed out coils
                                transients=transients,
                                uncorrelated=True)

    d = -4 if multicoil>1 else -3
    fidSum = torch.stack((fidSum.clone() + noise, fidSum), dim=d)
    spectral_fit = torch.stack((spectral_fit.clone() + noise,
                                spectral_fit), dim=d)

    # Keep both noisy transients and clean transients
    # output.shape: [bS, ON\OFF, [noisy/clean], transients, channels, length]
    #
```

## Modular Only

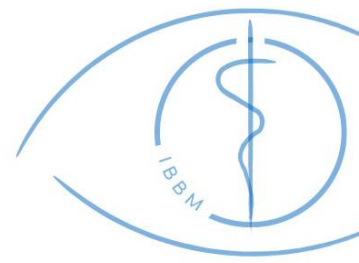
```
# Rephasing Spectrum
if phi0:
    fidSum = self.zero_order_phase(fid=fidSum,
                                    phi0=params[:,self.index['phi0']])

# Rephasing Spectrum
if phil:
    fidSum = self.first_order_phase(fid=fidSum,
                                    phil=params[:,self.index['phil']])

# Frequency Shift
if fshift_g:
    fidSum = self.frequency_shift(fid=fidSum,
                                   param=params[:,self.index['f_shift']])

# Eddy Currents
if eddy:
    fidSum = self.first_order_eddy_currents(fid=fidSum,
                                              params=params[:,self.index['ecc']])
```





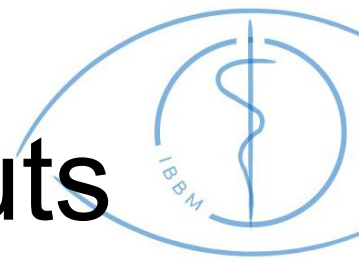
# Documentation

Documentation will help:

You with developing **your own** code **AND**

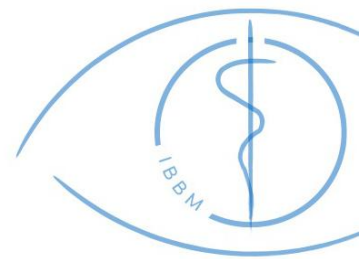
You and your collaborators to understand **each other's** code

What do we mean by “*documentation*”?



# Documentation - Describe inputs/outputs

```
def generate_noise(self, fid, param, max_val, zeros, transients, uncorrelated):  
  
def generate_noise(self,  
    fid: torch.Tensor,          # torch.Size([bS, (transients), channels, specLength])  
    param: torch.Tensor,        # torch.Size([bS])  
    max_val: torch.Tensor,      # max_val.ndim==fid.ndim  
    zeros: torch.Tensor,        # number of coils with no signal;  
                                # *coil sensitivities; torch.Size([bS, num_transients])  
    transients: torch.Tensor=None, # coil SNR values  
    uncorrelated: bool=True,    # correlate real/imaginary?  
    ) -> torch.Tensor:         # fid.shape
```



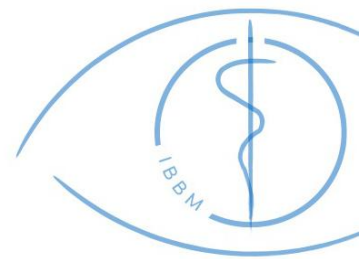
# Documentation - Explain the steps

```
# Load the simulated data
with open(datapath, 'r') as file:
    data = io.loadmat(file)
    specDataCmplx = data['spectra']
    header = data['header']

# Reshape data to fit into the container
x, y = reshape if not isinstance(reshape, type(None)) else 1, 1
z = specDataCmplx.shape[0] / (x*y)
s = specDataCmplx.shape[-1]
specDataCmplx = specDataCmplx.reshape(x,y,z,s)

# Define the metadata
json_full, meta_dict = self.set_metadata(name, header)

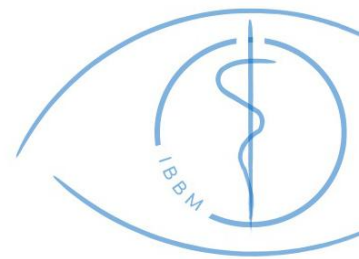
# Write the NIfTI files
self.write_NifTIMRS(specDataCmplx, self.currNiftiOrientation, header,
                    json_full, path, os.path.splitext(name)[0])
```



# Documentation - Important Details

```
# Define the delta values in each direction centered at 1 to avoid
# zeroing out values when centered at 0.
center = 1
# output.shape = [bS, 1, length, 1, 1]
x = batch_linspace(center-dx,center+dx,num_pts[0]).permute(0,2,1).unsqueeze(-1)
# output.shape = [bS, 1, 1, length, 1]
y = batch_linspace(center-dy,center+dy,num_pts[1]).unsqueeze(-1)
# output.shape = [bS, 1, 1, 1, length]
z = batch_linspace(center-dz,center+dz,num_pts[2]).unsqueeze(-1).permute(0,1,3,2)

# Define the changes in B0
dB0 = x * x.transpose(-3,-2) / dx.unsqueeze(-1) # output.shape = [bS, 1, length, length, 1]
dB0 += y
dB0 = dB0.repeat(1,1,1,z.shape[-1]) + z # output.shape = [bS, 1, length, length, length]
dB0 += mean - center
# dB0.shape = [bS, 1, length, length, length]
```



# Documentation - Describe your files

```
1 → % op_autophase.m
2 → % Jamie Near, McGill University 2015.
   %
3 → % USAGE:
   % [out,phaseShift]=op_autophase(in,ppmmin,ppmmax,ph,dimNum);
   %
4 → % DESCRIPTION:
   % Search for the peak located between ppmmin and ppmmax, and then phase the
   % spectrum so that that peak reaches the desired phase.
   %
5 → % INPUTS:
   % in          = input data in matlab structure format.
   % ppmmin      = minimum of ppm search range.
   % ppmmax      = maximum of ppm search range.
   % ph          = desired phase value in degrees [optional. Default=0].
   % dimNum      = which subSpec dimension to use for phasing? [Only for use in data with multiple subSpectra].
   %
6 → % OUTPUTS:
   % out         = Output following automatic phasing.
   % phaseShift  = The phase shift (in degrees) that was applied.
```

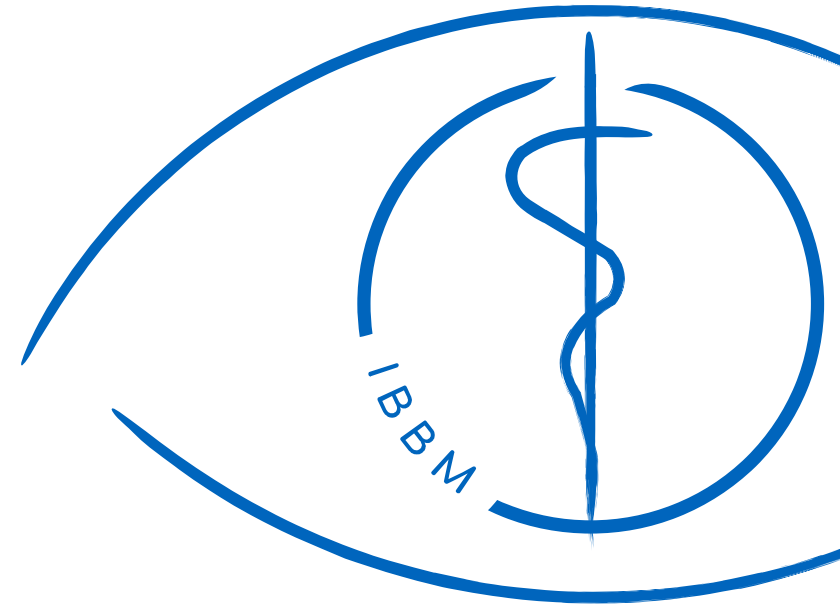
## Osprey Example

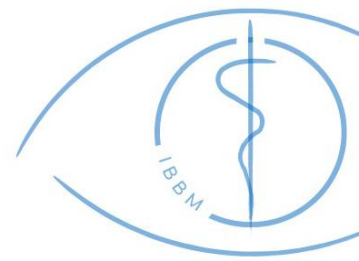
1. File name
2. Author
3. Function call
4. Description
5. Inputs
6. Outputs

# Questions?

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Happy Hacking!





# Example: Data Simulator

## Starting Point

### Steps:

1. Write code for entire model
- 2: Test code
- 3: Publish code

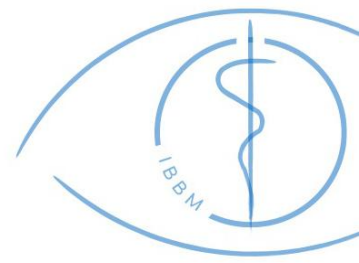
Essentially true, yes, but...

- Poorly thought out
- No concrete steps
- No clear starting point

## Better Developed

### Steps:

1. Sketch outline for approach
  - E.g. 1 sample at a time or batches?
  - What is the bare minimum?
  - Order of operations
- 2: Write code for bare minimum example
  - Load basis set
  - Modulate and sum basis functions
  - Save outputs



# Efficiency

- Mentioning for completeness
- Keep in mind how the required computational resources change
- Efficiency can be optimized to different levels
- Basic efficiency should be kept in mind during development
- Optimization should be done towards the end