Using the VAMPIRE Data Converter

Installation

- VAMPIRE source:
  https://github.com/richard-evans/vampire.git
  Use “develop” branch

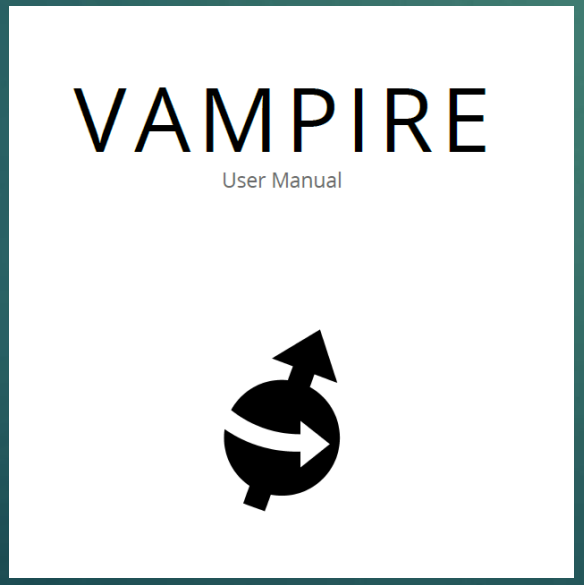
- In terminal:
  `make vdc`

- The vdc executable can then be found at:
  `…/vampire/util/vdc/vdc`

The Manual

- Included in the source under `…/vampire/manual/vampire-manual.tex`

- A LaTeX file must be compiled into a pdf



Displaying Atomic positions

- Requires input file parameter:

  `config:atoms`

- This must be included before running the simulation
  - New files: data and meta files

- Run vdc:
  `util/vdc/vdc -xyz`
  - `New file: crystal.xyz`

- `Use a .xyz file viewer such as Jmol or VESTA`

Customisation and Troubleshooting

- VDC should also be used to check inputs
- Using slices
  - `--slice [`x_{min}`,` x_{max}`,` y_{min}`,` y_{max}`,` z_{min}`,` z_{max}`]`
  - Parameters are in fractional coordinates
- `Removing materials`
  - *`--remove-material [material1,material2,...]`*
  - *Material numbers correspond to those in material file*
- *More options are explained in the Manual*

Displaying Spins in POV-Ray

- Initial requirements:
  - Use `config:atoms`
  - POV-Ray installation
    - Ubuntu: `sudo apt install povray`
    - Otherwise find binaries at http://povray.org/download/
- Run vdc:
  - `utils/vdc/vdc --povray`
  - `Several new files: .inc .ini .pov`

POV-Ray Customisation

- The spins.pov file:

```
//-------------------------------------------------------------
// Povray file generated using vampire
//-------------------------------------------------------------
#version 3.5;
#include "colors.inc"
#include "metals.inc"
#include "screen.inc"
#declare LX=0.0;
#declare LY=0.0;
#declare LZ=0.0;
#declare CX=300.008;
#declare CY=600.005;
#declare CZ=150.006;
#declare ref=0.05;
global_settings { assumed_gamma 2.0 }
background { color Gray30 }
Set_Camera(<CX,CY,CZ>, <LX,LY,LZ>, 15)
Set_Camera_Aspect(4,3)
Set_Camera_Sky(<0,0,1>)
```

Look at Position

Camera Position

Camera Angle

Displaying Spins in POV-Ray

- To run povray:
  `povray -w3600 -h2700 +A0.3 spins`

- `-w` and `-h` choose the image width and height (resolution) and +A0.3 uses antialiasing.

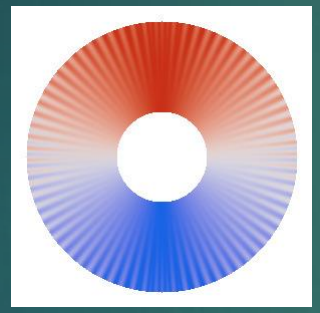
- `The spins.pov file contains additional options`

POV-Ray Customisation

- Command line parameters:
  - `--vector-z [x,y,z]` to change primary axis
  - --colourmap [name] to change palette
- Some colourmaps lend themselves better to different systems
  - For Vortex systems try “C2”

POV-Ray Colourmaps

- Default: Red-White-Blue-White-Red



- Other options:
  - For vortex: C2