

OpenDIEL Software Development and GUI

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How does openDIEL work?

- openDIEL is a wrapper to schedule work on a set of resources (workflow engine)
- Create a driver program in C
- Create a makefile
- Create modules to be run
- Create workflow.cfg file
- Execute mpirun (calculate number of processes)



Functionalities of GUI

- GUI seeks to eliminate some of the tasks in this tedious process
- Load module
- Create workflow
- Calculate number of processes
- Call mpirun system command



GUI

Welcome | Module Specification | Workflow | Machine Learning | LIGGGHTS | Save | Launch

New Module

Module Type Managed Automatic

Library Type Static Dynamic

Module Name

Path To Library

Path to include:

Input Arguments

Boundary Points

Size

Copies

Processes Per Co

Threads Per Proc

Number of GPUs

Split Directory

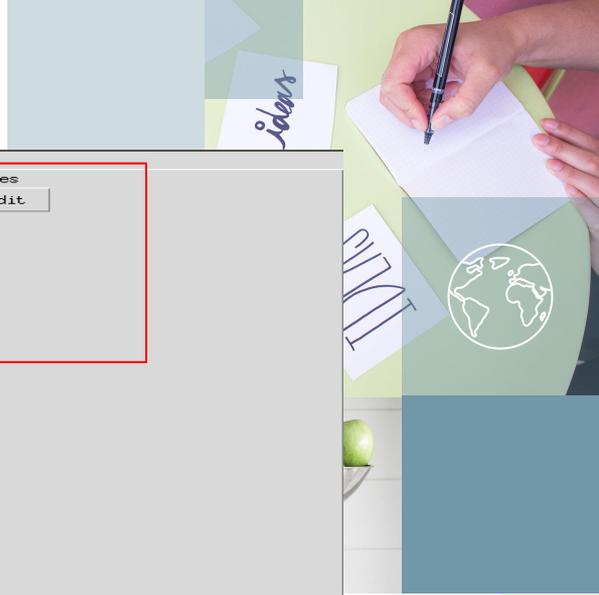
Saved Modules

omartest

Load Existing Modules

Preconfigured Modules

-
-
-
-
-
-
-
-



GUI



Welcome | Module Specification | Workflow | Machine Learning | LIGGGHTS | Save | Launch

New Module

Module Type

Library Type

Module Name

Path To Library

Path to include:

Input Arguments

Boundary Points

Size

Copies

Processes Per Co

Threads Per Pro

Number of GPUs

Split Directory

Saved Modules

MODULE-0	<input type="button" value="Edit"/>
MODULE-1	<input type="button" value="Edit"/>
MODULE-2	<input type="button" value="Edit"/>
MODULE-3	<input type="button" value="Edit"/>
MODULE-4	<input type="button" value="Edit"/>
!TupleServe	<input type="button" value="Edit"/>

<input type="button" value="Load test_module"/>
<input type="button" value="Load optimize"/>
<input type="button" value="Load first"/>
<input type="button" value="Load second"/>
<input type="button" value="Load third"/>
<input type="button" value="Load fourth"/>
<input type="button" value="Load fifth"/>
<input type="button" value="Load last"/>

GUI

Welcome | Module Specification | Workflow | Machine Learning | LIGGGHTS | Save | Launch

Available Modules

MODULE-0	Add To Group
MODULE-1	Add To Group
MODULE-2	Add To Group
MODULE-3	Add To Group
MODULE-4	Add To Group
ielTupleServer	Add To Group

Available Groups

g1	Edit	Add Dependency
g2	Edit	Add Dependency

Load Workflow from File

New Group

Group Name

Modules to run

Iterations

Dependencies

Save Group

```
workflow =
{
  tuple_set =
  {
    tuple_group =
    {
      order =
      (
        "ielTupleServer"
      );
      iterations = 1;
    };
  };
  main_set =
  {
    g1 =
    {
      order =
      (
        "MODULE-1",
        "MODULE-2",
        "MODULE-3"
      );
      iterations = "1";
    };
  };
};
```



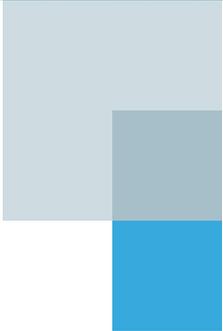
GUI



Welcome | Module Specification | Workflow | Machine Learning | LIGGGHTS | Save | Launch |

CFG File Name

```
tuple_space_size = 0;
number_of_gpu = 1;
modules =
{
  MODULE-0 =
  {
    function = "MODULE-1";
    args =
    {
      "'../helloiexe'");
    };
    size = 5;
    libtype = "static";
  };
  MODULE-1 =
  {
    function = "MODULE-1";
    args =
    {
      "../helloiexe"
    };
    size = 5;
    libtype = "static";
  };
  MODULE-2 =
  {
    function = "MODULE-3";
    args =
    {
      "'../helloifexe'");
  }
```



GUI

Welcome | Module Specification | Workflow | Machine Learning | LIGGGHTS | Save | Launch

Example Workflows

Launch Fantest

Display Attribute Info.

Defined Workflow

Output Directory |

Output Directory Location



Challenges we faced

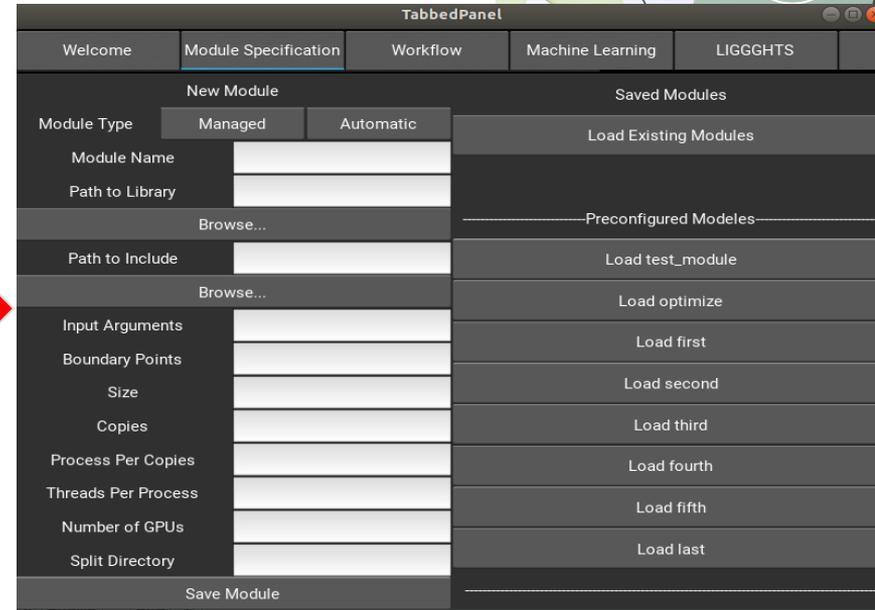
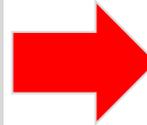
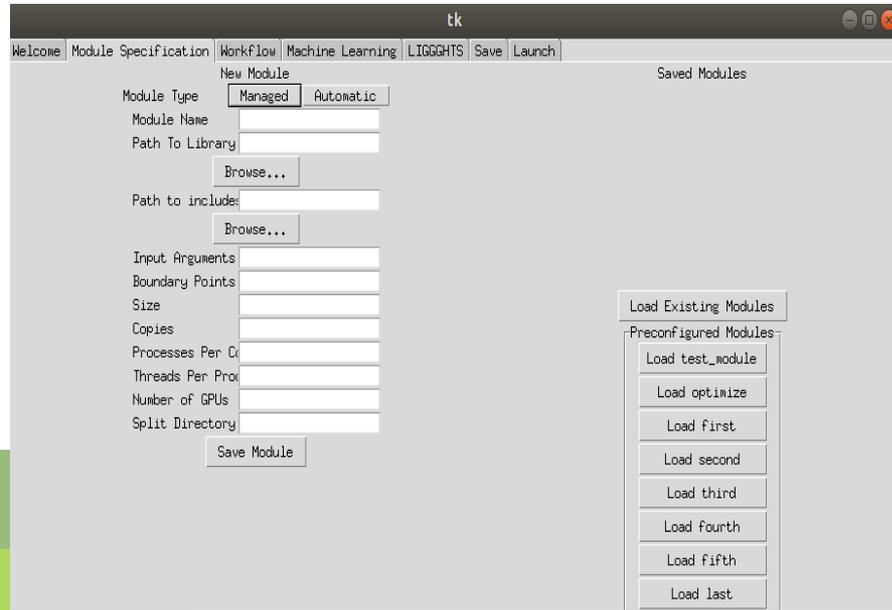
- Syntax Errors
- Understanding the code
- Configuration file formatting
- Semantic Errors
- Loading modules created using the GUI
- Launching mpirun command from non-source directory
- Design issues

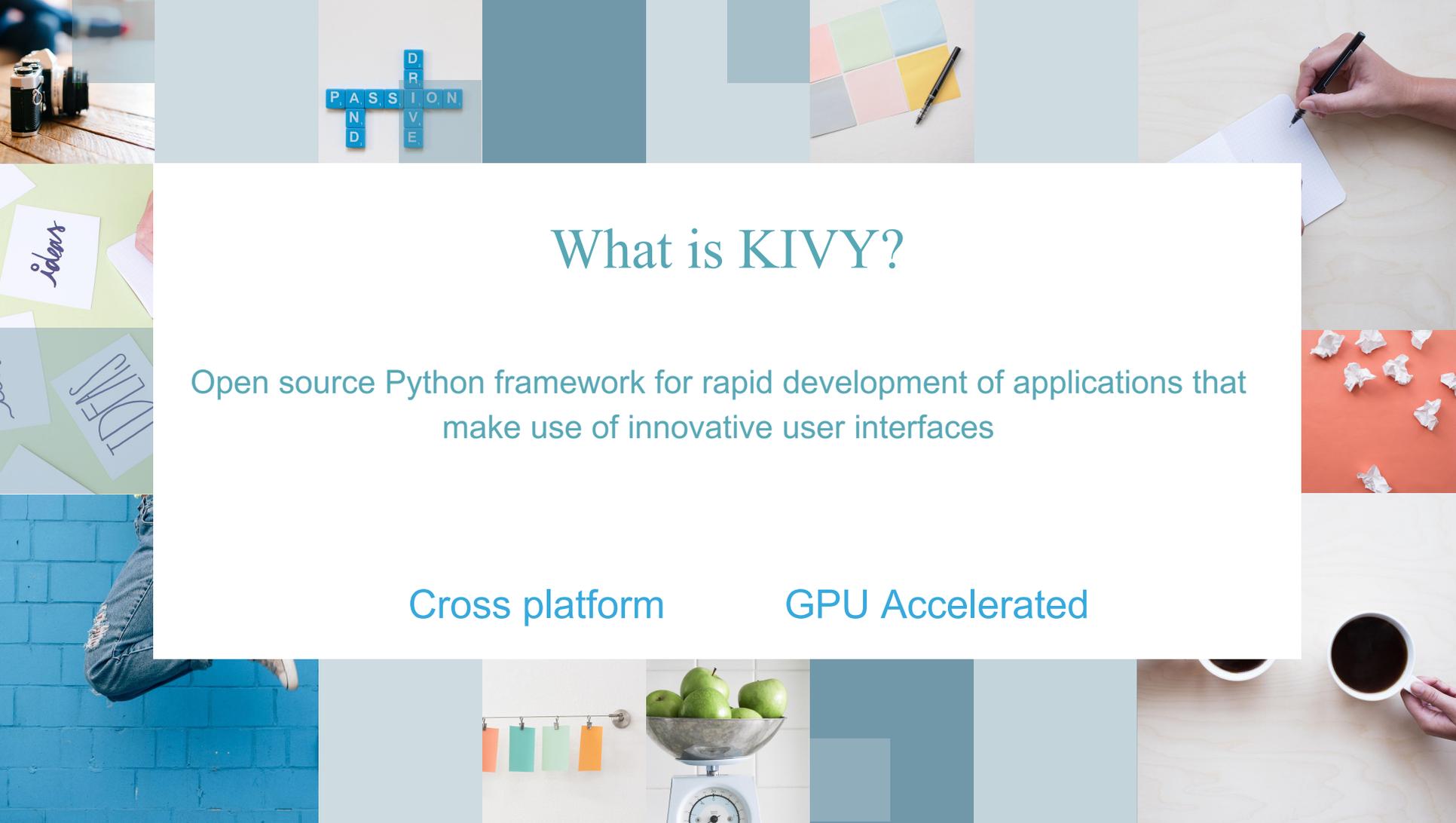


Future Development

Tkinter

KIVY





What is KIVY?

Open source Python framework for rapid development of applications that make use of innovative user interfaces

Cross platform

GPU Accelerated

Why KIVY?

Tkinter:

outdated

not visually appealing

KIVY :

all intensive purposes

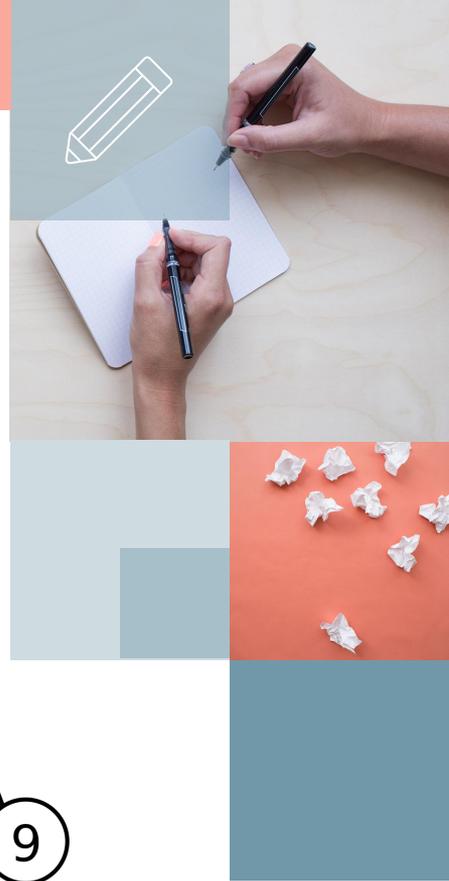
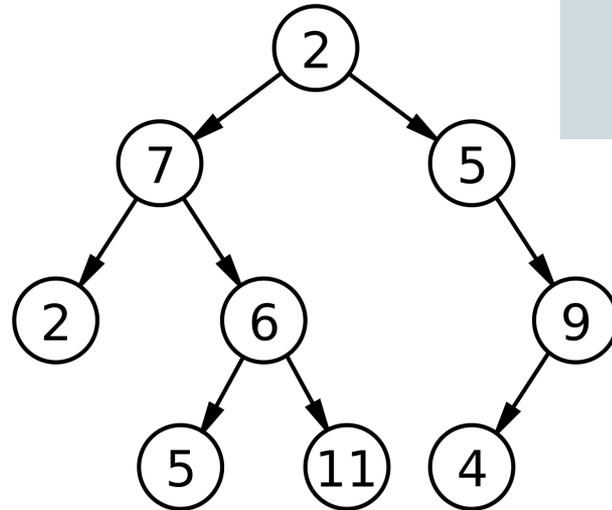
>design language

mobile app development



How does KIVY work?

- Must be familiar with python
- KV language which allows you to create your widget tree in a declarative way
- bind widget properties to each other or to callbacks in a natural manner



Differences in KIVY vs. Tkinter

- Tkinter
 - desktop focused
- KIVY
 - automatically formats widgets to most appealing design
 - works across all platforms
 - special language for defining layout. This allows you to keep your logic and presentation separate. (Ex. CSS and HTML)



```
1 #Kivy 1.1.0
2
3 Root:
4   text_input: text_input
5
6   BoxLayout:
7     orientation: 'vertical'
8     Widget:
9       size_hint_y: None
10      height: 30
11      Button:
12        text: 'Load'
13        on_release: root.show_load()
14      Button:
15        text: 'Save'
16        on_release: root.show_save()
17
18   BoxLayout:
19     TextInput:
20       id: text_input
21       text: ''
22
23     MDocument:
24       text: text_input.text
25       show_errors: True
26
27 <loadDialog>:
28   BoxLayout:
29     size: root.size
30     pos: root.pos
31     orientation: 'vertical'
32     FileChooserIconView:
33       id: filechooser
34
35   BoxLayout:
36     size_hint_y: None
37     height: 30
38     Button:
39       text: 'Cancel'
40       on_release: root.cancel()
41
42     Button:
43       text: 'Load'
44       on_release: root.load(filechooser.path, filechooser.selection)
45
46 <saveDialog>:
47   text_input: text_input
48   BoxLayout:
```

How is Kivy going now

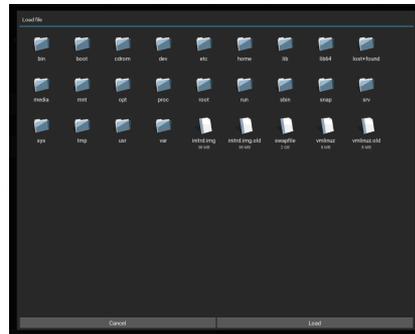
- GUI (done)
- functionality (currently working on it)
 - Hide and show widget (done)
 - browse file (finished, need improvement[bugs fixed, better searching engine & GUI])



```
class Person:
    def __init__(self, firstName, familyName):
        self.first = firstName
        self.familyName = familyName

    def fullName(self):
        return "{} {}".format(self.first, self.familyName)

def main():
    print("Hello world!")
    firstName = "Frankie"
    familyName = "Betancourt"
    classInstance = Person(firstName, familyName)
    classInstance2 = Person("John", "Smith")
    fullName = classInstance.fullName()
    fullName2 = classInstance2.fullName()
    print("{} {}".format(fullName))
    print("{} {}".format(fullName2))
    main()
```



```
class Person:
    def __init__(self, firstName, familyName):
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        self.familyName = familyName

    def fullName(self):
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def main():
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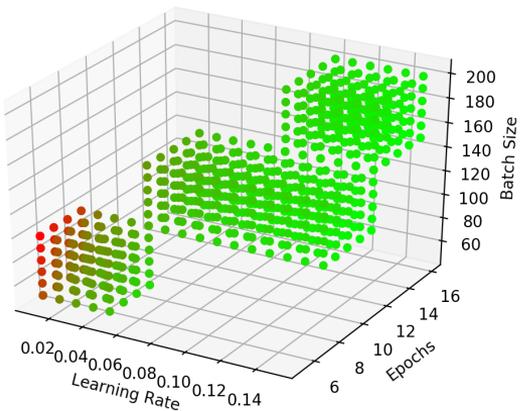
    classInstance = Person(firstName, familyName)
    classInstance2 = Person("John", "Smith")

    fullName = classInstance.fullName()
    fullName2 = classInstance2.fullName()

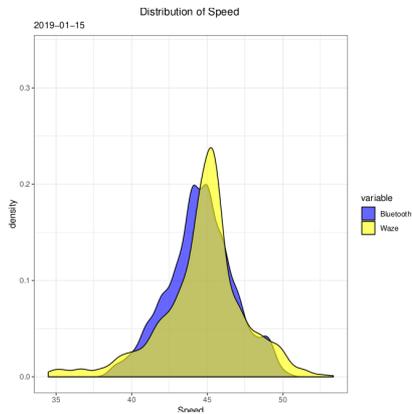
    print("{} {}".format(fullName))
    print("{} {}".format(fullName2))
    main()
```

Applications of openDIEL

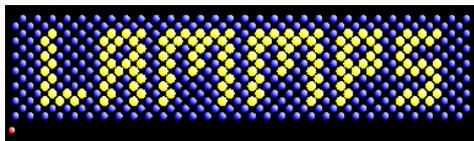
Grid Engine with MagmaDNN



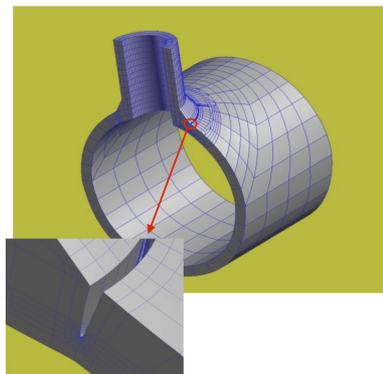
Traffic Flow Data Analytics



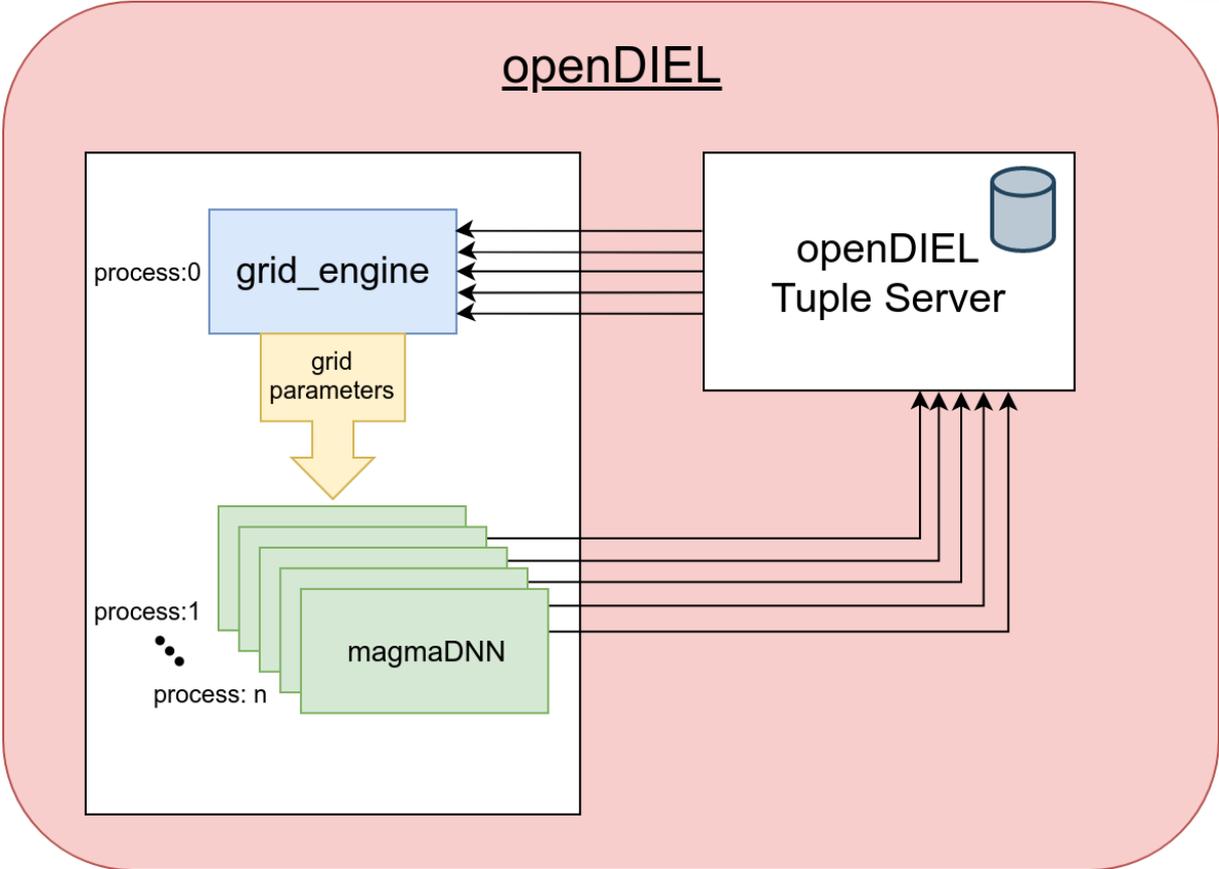
Computational Chemistry of Epoxy System



Computational Mechanics: Warp 3D



Example Workflow: MagmaDNN Grid Engine



Research Goal

Fully functional GUI on KIVY to provide a stylish, user-friendly platform to help use openDIEL





PASSION
DRIVE
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Any Questions?