

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

GUI

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

New Module

Module Type: ☐ Managed ☐ Automatic

Library Type: ☐ Static ☐ Dynamic

Module Name: omartest

Path To Library:

Path to include:

Input Arguments: python tmp.py

Boundary Points:

Size:

Copies:

Processes Per Co:

Threads Per Proc:

Number of GPUs: 1

Split Directory:

Saved Modules

omartest

Load Existing Modules

Preconfigured Modules

A crossword puzzle grid is shown. The word "PASSION" is written across the middle, and the word "DROVE" is written vertically down the center, intersecting "PASSION" at the letter "O". The letters are on blue tiles with white numbers. The grid is set against a light gray background.

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:

```

graph TD
    A[Load Existing Modules] --> B[Preconfigured Modules]
    B --> C[Load test_module]
    B --> D[Load optimize]
    B --> E[Load first]
    B --> F[Load second]
    B --> G[Load third]
    B --> H[Load fourth]
    B --> I[Load fifth]
    B --> J[Load last]
  
```

GUI

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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	<input type="text"/>
Modules to run	<input type="text"/>
Iterations	<input type="text"/>
Dependencies	<input type="text"/>

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 WorkflowAM.cfg

Create Configuration File

```
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',
    );
```

D
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GUI

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

Example Workflows

Launch Fantest

Display Attribute Info.

Defined Workflow

Output Directory |

Output Directory Location Browse...

Launch Job



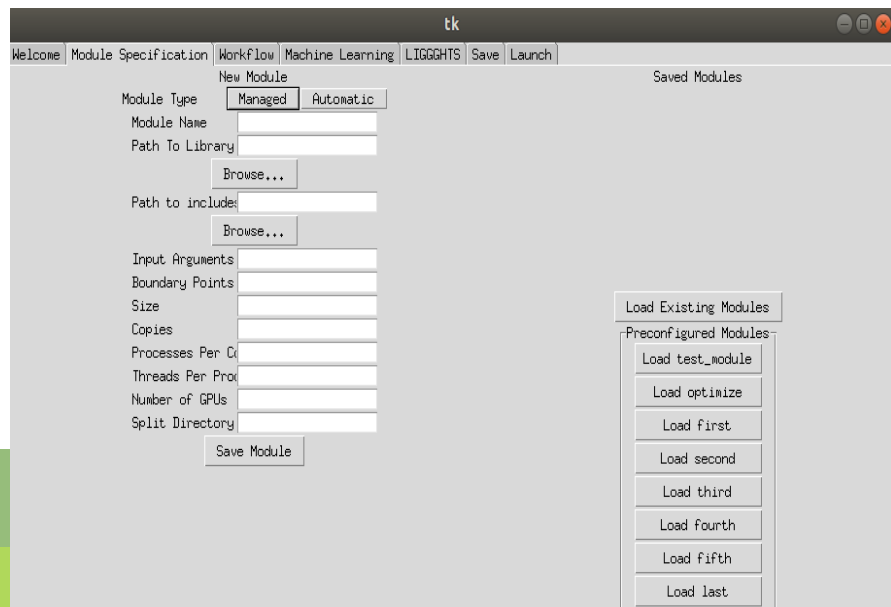
Challenges we faced

- 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

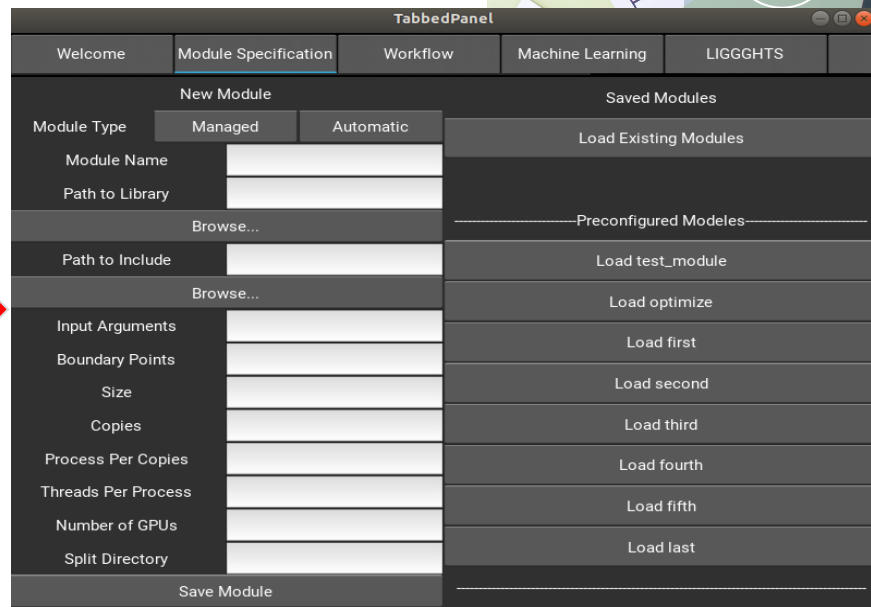


Future Development

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

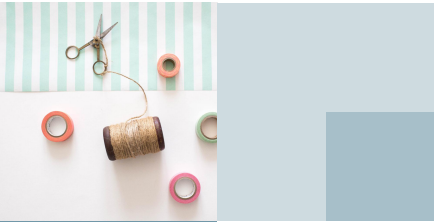
not visually appealing

KIVY :

all intensive purposes

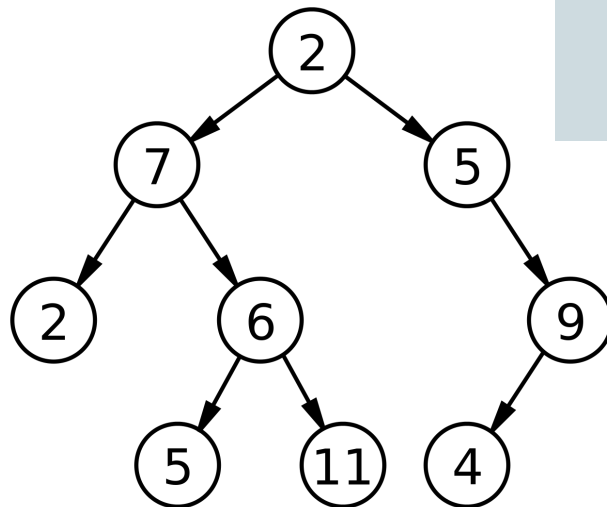
>design language

mobile app development



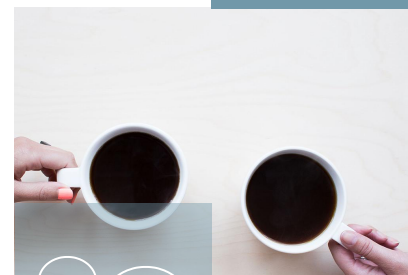
How does KIVY work?

- 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

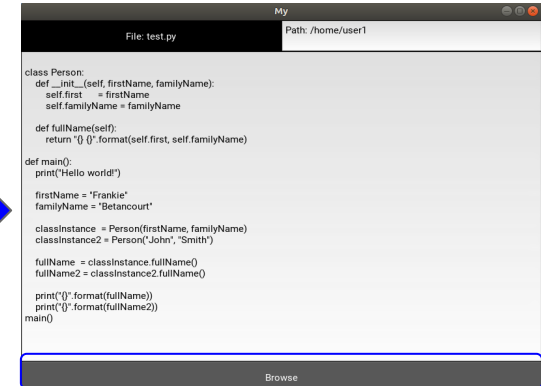
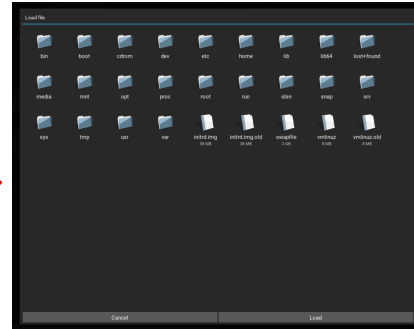
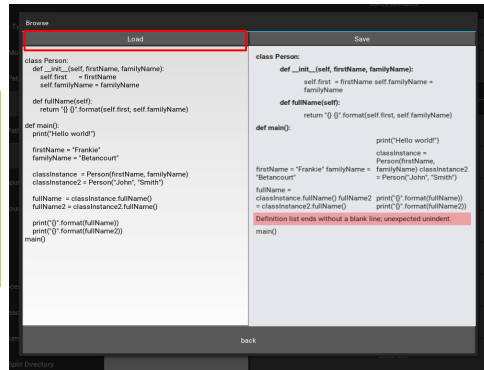
- Tkinter
 - desktop focused
- KIVY
 - automatically formats widgets to most appealing design
 - works across all platforms
 - special language for defining layout. This allows you to keep your logic and presentation separate. (Ex. CSS and HTML)



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

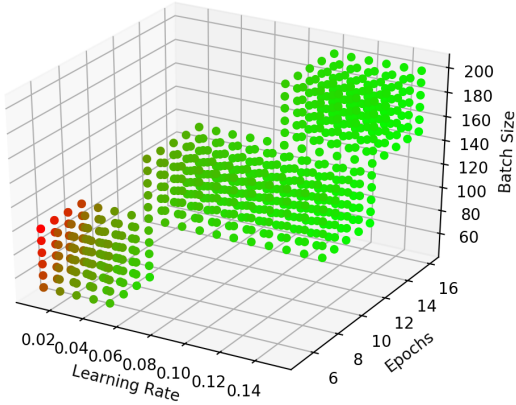
How is Kivy going now

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

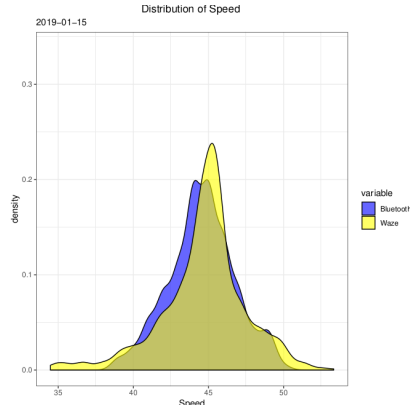


Applications of openDIEL

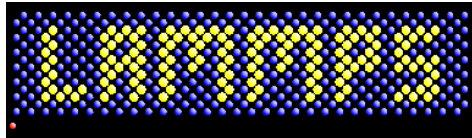
Grid Engine with MagmaDNN



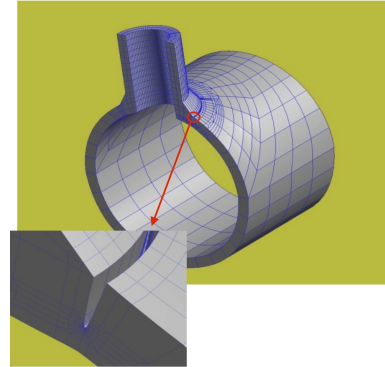
Traffic Flow Data Analytics



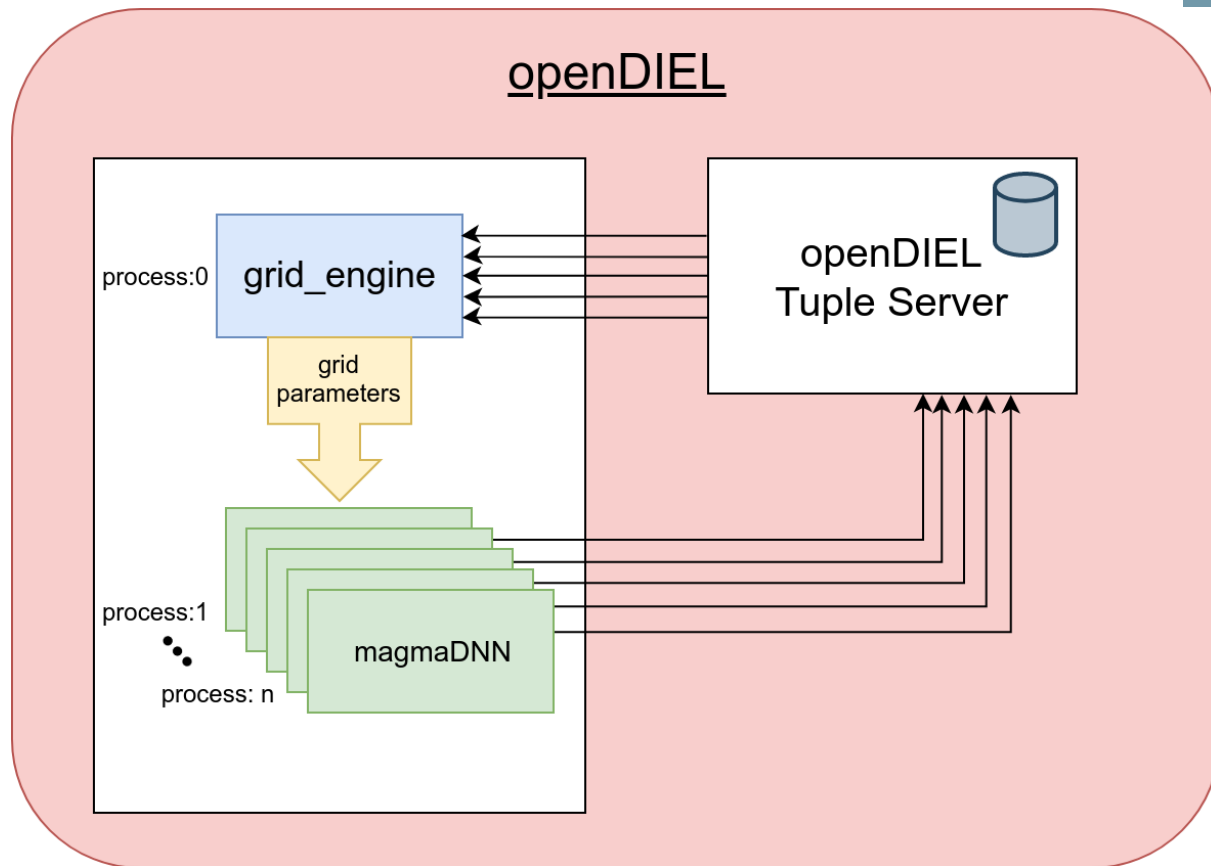
Computational Chemistry of Epoxy System



Computational Mechanics: Warp 3D



Example Workflow: MagmaDNN Grid Engine



PASSION
DRIVE



Research Goal

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





Any Questions?