MMODEL

modular modeling framework for scientific prototyping

modular
- DAG workflow
- based on networkx

lightweight
- function as node

distributable
- with graph or model

customizable
- wrapper as modifier

addresses:
- different programming proficiencies
- rapid prototyping
- difficulties in unit tests

Peter Sun, John Marohn
Department of Chemistry and Chemical biology, Cornell University

Overview

```python
def func_a(x, y):
    return x + y


def func_b(sum_xy, z):
    return math.log(sum_xy, z)


def func_c(sum_xy, log_xy):
    return sum_xy * log_xy


doc = """MModel example function
calculates the mathematical formula (x + y)log(x + y, z)
"""
graph = ModelGraph(name="Example", doc=doc)

grouped_edges = [("func a", ["func b", "func c"]), ("func b", "func c")]
graph.add_grouped_edges_from(grouped_edges)

node_objects = [
    ("func a", func_a, ["sum_xy"]),
    ("func b", func_b, ["log_xy"]),
    ("func c", func_c, ["result"]),
]
graph.set_node_objects_from(node_objects)

example_func = Model(graph, handler=MemHandler)
```

define functions

define graph

define nodes and edges

link nodes to functions

define model

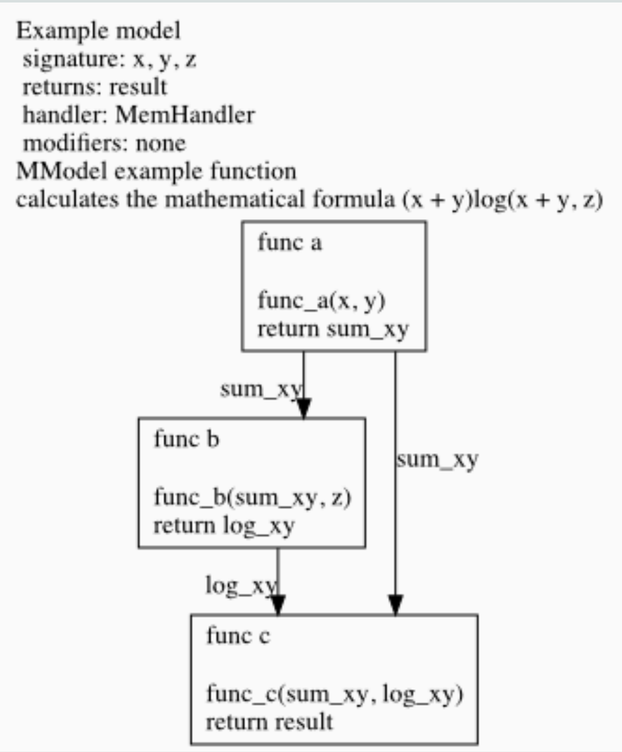
```
>>> print(example_func)
Example model
  signature: x, y, z
  returns: result
  handler: MemHandler
  modifiers: none
MModel example function
Calculates the mathematical formula (x + y)log(x + y, z)

>>> example_func(5, 3, 2) # (5 + 3)log(5 + 3, 2)
24.0

>>> example_func.draw() # draw model graph
```

MModel components

graph: outlines DAG workflow (networkx based)
handler: handles graph execution
modifier: decorates graphs, subgraphs, or nodes
model: creates workflow callables



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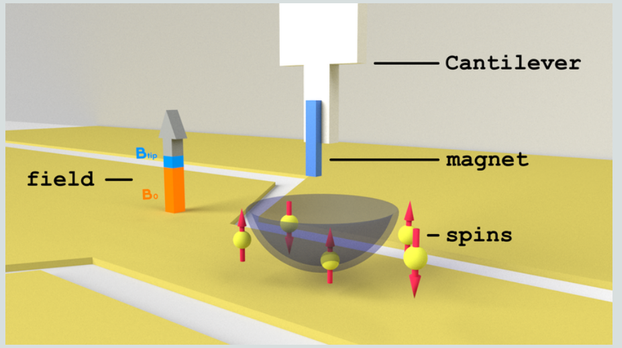
Building scientific packages using mmodel (developer)

mrfmsim

Simulate signals in Magnetic Resonance Force Microscope experiments



Create a new experiment:

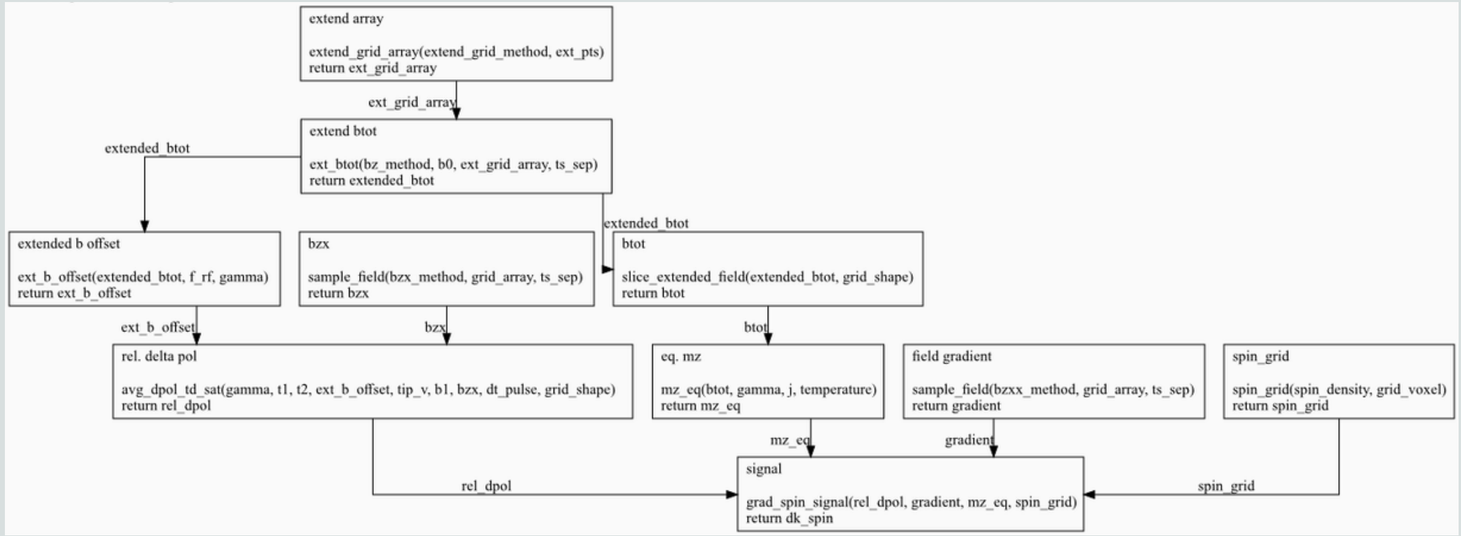
```python
from mmodel import ModelGraph
from mrfmsim.function import ...

grouped_edge_list = [
    ("extend array", "extend btot"),
    ("extend btot", ["extended b offset", "btot"]),
    ("btot", "eq. mz"),
    (["bzx", "extended b offset"], "rel. delta pol"),
    (["eq. mz", "field gradient", "rel. delta pol", "spin_grid"], "signal"),
]

td_esr_graph = ModelGraph(doc=doc, name = "td_esr")
td_esr_graph.add_grouped_edges_from(grouped_edge_list)
```

```python
node_objects = [
    ("extend array", extend_grid_array, ["ext_grid_array"]),
    ("extend btot", ext_btot, ["extended_btot"]),
    ("btot", slice_extended_field, ["btot"]),
    ("bzx", sample_field, ["bzx"], [smod(["bzx_method", "grid_array", "ts_sep"])]),
    ("field gradient", sample_field, ["gradient"]),
    ("eq. mz", mz_eq, ["mz_eq"]),
    ("rel. delta pol", avg_dpol_td_sat, ["rel_dpol"]),
    ("extended b offset", ext_b_offset, ["ext_b_offset"]),
    ("spin_grid", spin_grid, ["spin_grid"]),
    ("signal", grad_spin_signal, ["dk_spin"]),
]

td_esr_graph.set_node_objects_from(node_objects)
ts_esr_model = Model(td_esr_model, handler=MemHandler, modifiers=[])
```



Developer role

1. define functions
2. **define experiment graphs with functions**
3. **define default models**
4. test functions and models
5. define shortcuts and additional modifiers

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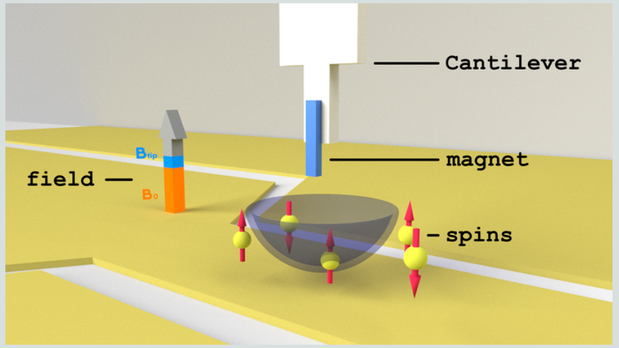

Create a package-specific shortcut:

mmodel
```
subgraph = subgraph_by_parameters(graph, ["b0"])
loop_node = Model(subgraph, MemHandler, [loop_modifier("b0")])
looped_graph = modify_subgraph(graph, subgraph, "b0 loop node", loop_node)
looped_model = Model(looped_graph, handler=MemHandler)
```

mrfmsim
```
looped_model = loop_shortcut(td_esr_model, "b0")
```

mrfmsim
```
from mmodel import Model, subgraph_by_parameters, modify_subgraph, loop_modifier

def loop_shortcut(model, loop_parameter: str):
    """Shortcut to add loop to subgraph of the given model

    :return: a new model that loops the parameter in the subgraph
    """
    loop_mod = loop_modifier(loop_parameter)
    handler = model._handler
    graph = model._graph
    model_modifiers = model._modifiers
    node_name = f"{loop_parameter} loop node"

    subgraph = subgraph_by_parameters(graph, [loop_parameter])
    loopee_node = Model(subgraph, handler, loop_mod)
    looped_graph = modify_subgraph(graph, subgraph, node_name, loop_node)
    looped_model = Model(looped_graph, handler)

    return looped_model
```

Modify a subgraph in mmodel

1. find the subgraph
2. create a "function" (model) base on subgraph
3. substitute graph with a "submodel"
4. create a new model based on the new graph

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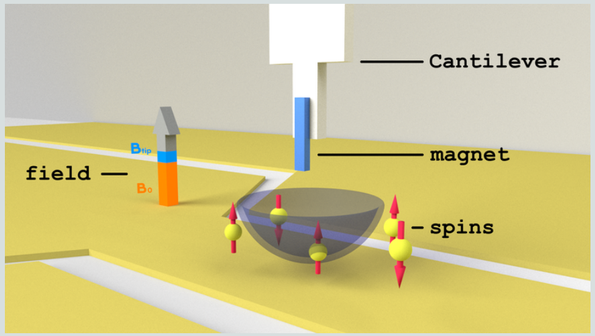


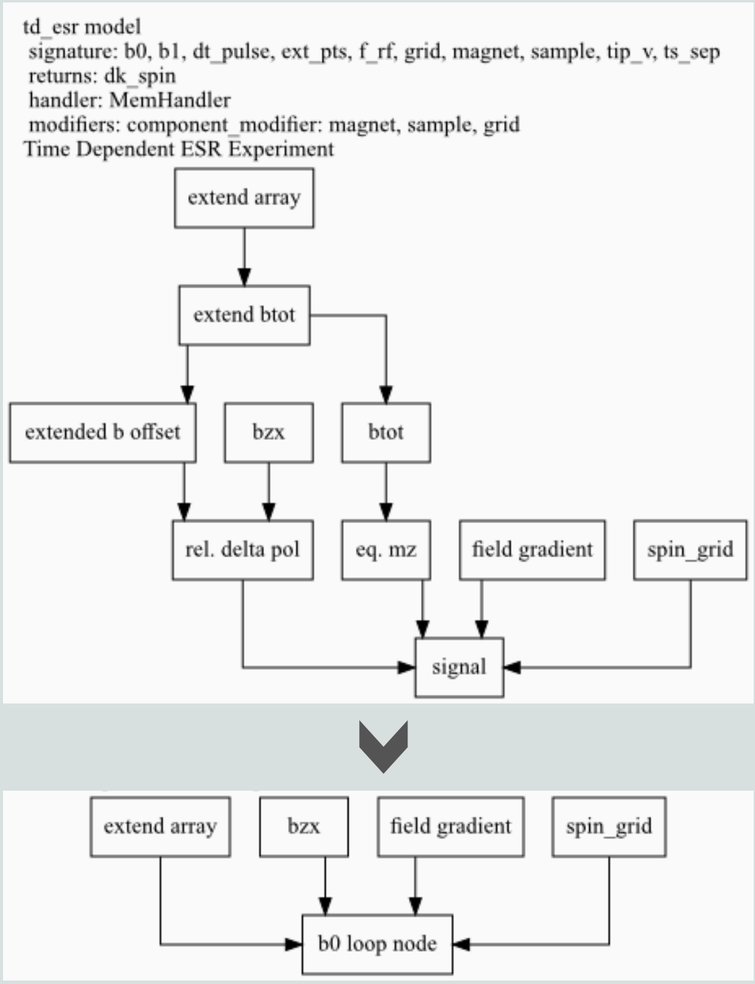
Create a loop in model and execute the model:

```python
from mmodel import draw_plain_graph
from mrfmsim.shortcut import loop_shortcut
from mrfmsim.experiment import td_esr_model

td_esr_model.draw(method=draw_plain_graph)

td_esr_b1_looped_model = loop_shortcut(td_esr_model, "b1")

dk_spin_td_b1loop = td_esr_b1_looped_model(
    dt_pulse=5.44e-4,
    grid=grid,
    magnet=magnet,
    sample=sample,
    ts_sep=[0, 150.0, 0],
    b1=b1_list,
    f_rf=18.1e9,
    b0=645,
    ext_pts=[x_pts, 0, 0],
    tip_v=tip_v,
)
```



User role

1. Inspect model graph
2. Modify model or subgraph using modifiers
3. Execute model as a function