Automating GPU adaptation of NWP single column physics using Loki

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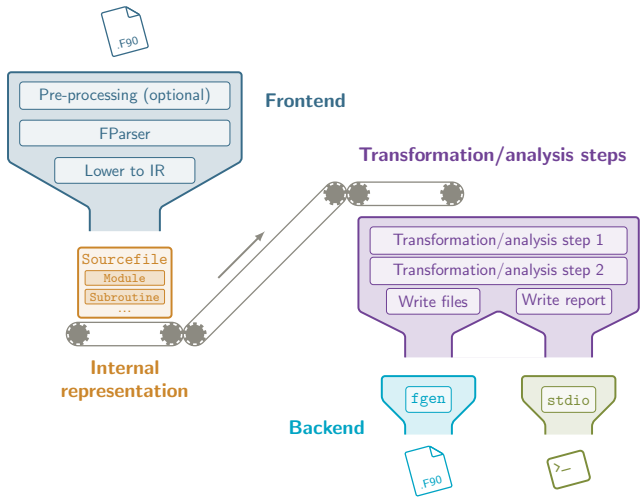
Introduction

- Michael S. just gave us an in-depth explanation of how NWP single column algorithms can be adapted to optimally exploit GPU hardware
- The current talk focuses on Loki, our source-to-source translation tool used to automate this adaptation

Loki - source-to-source translation tool

- **Loki** - programmable source-to-source translation toolchain for Fortran codes
- Written in Python
- Typical Loki pipeline:



Loki - parsing

- First parsing step: use *Fparser*[1] to obtain an abstract syntax tree (AST)
  - Supports all of F2003, F2008 features added regularly
- AST enriched with context and metadata to form a custom internal representation (IR)

Parse expression-tree

```
>>> from loki import parse_fparser_expression, Scope
>>> expr = parse_fparser_expression('a*(b*(c+(d+e)))',
...                                 scope=Scope())
>>> print(expr)
a*(b*(c + (d + e)))
>>> type(expr)
<class 'loki.expression.symbols.Product'>
```

Parse sourcefile

```
>>> from loki import Sourcefile
>>> source = Sourcefile.from_file('src/phys_mod.F90',
...                               preprocess=True)
>>> type(source)
<class 'loki.sourcefile.Sourcefile'>
>>> len(source.modules)
1
>>> len(source.subroutines)
0
```

Parse subroutine

```
>>> from loki import Subroutine
>>> fcode = """subroutine add_ints(a,b,c)
... implicit none
... integer, intent(in) :: a,b
... integer, intent(out) :: c
...
... c = a+b
... end subroutine add_ints"""

>>> routine = Subroutine.from_source(fcode)
>>> type(routine)
<class 'loki.subroutine.Subroutine'>
>>> print(routine.name)
'add_ints'
>>> len(routine.arguments)
3
```

Loki - IR

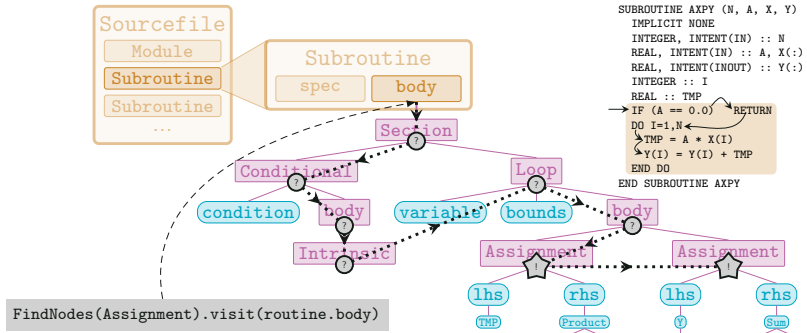
- Fortran language constructs are stored as individual IR nodes

```
### extract module from src/phys_mod.F90
>>> phys_mod = source['phys_mod']
>>> phys_mod
Module:: phys_mod
>>> from loki import fgen
>>> print(fgen(phys_mod.spec))
USE iso_fortran_env

USE omp_lib

IMPLICIT NONE

INTEGER, PARAMETER :: sp = REAL32
INTEGER, PARAMETER :: dp = REAL64



INTEGER, PARAMETER :: lp = dp!! lp : "local" precision


INTEGER, PARAMETER :: ip = INT64

REAL(KIND=lp) :: cst1 = 2.5, cst2 = 3.14
INTEGER, PARAMETER :: nspecies = 5
```

```
>>> phys_mod.spec.view()
<Section::>
  <Import:: iso_fortran_env => ()>
  <Comment:: >
  <Import:: omp_lib => ()>
  <Comment:: >
  <Intrinsic:: IMPLICIT NONE>
  <Comment:: >
  <VariableDeclaration:: sp>
  <VariableDeclaration:: dp>
  <CommentBlock:: >
  <VariableDeclaration:: lp>
  <CommentBlock:: >
  <VariableDeclaration:: ip>
  <Comment:: >
  <VariableDeclaration:: cst1, cst2>
  <VariableDeclaration:: nspecies>
```

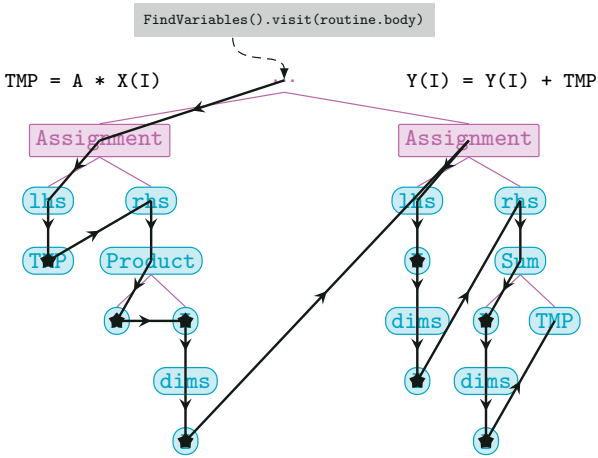
Loki - IR

- The Loki IR consists of two levels:
  - Outer level corresponds to control-flow nodes, e.g. `Assignment`, `Loop` (purple nodes)
  - Inner level corresponds to expression nodes, e.g. `Scalar`, `Array`, `Product` (blue nodes)
    - Built on top of the *Pymbolic*[2] library



Loki - visitors

- The previous slide showed an example of the `FindNodes` visitor utility to lookup control-flow nodes
- Loki relies heavily on visitor utilities to traverse/modify the IR
- Analogous utilities also exist for expression nodes, e.g. `FindVariables`



Loki - adding new functionality

- Extend functionality of `FindNodes` to create `FindNodesDepth` visitor
  - Perform node lookup *and* retrieve depth of node in IR

```python
from loki import FindNodes

class FindNodesDepth(FindNodes):

    def __init__(self, match, greedy=False):
        super().__init__(match, mode='type', greedy=greedy)


    # copied from FindNodes.visit_Node
    def visit_Node(self, o, **kwargs):
        ret = kwargs.pop('ret', self.default_retval())
        depth = kwargs.pop('depth', 0)
        if self.rule(self.match, o):
            ret.append((o, depth))
            if self.greedy:
                return ret
        for i in o.children:
            ret = self.visit(i, depth=depth+1, ret=ret, **kwargs)
        return ret or self.default_retval()
```

- `FindNodesDepth` can be created by changing only 4 lines of `FindNodes`

Loki - adding new functionality

- Apply both visitors to `SUBROUTINE AXPY` from earlier example

`FindNodes`

```
>>> from loki import Assignment, Subroutine, FindNodes
>>> routine = Subroutine.from_source(...)
>>> assigns = FindNodes(Assignment).visit(routine.body)
>>> len(assigns)
2
>>> print(assigns[0])
Assignment:: tmp = a*x(i)
```

`FindNodesDepth`

```
>>> from loki import Assignment, Subroutine, FindNodesDepth
>>> routine = Subroutine.from_source(...)
>>> assigns = FindNodesDepth(Assignment).visit(routine.body)
>>> len(assigns)
2
>>> print(assigns[0])
(Assignment:: tmp = a*x(i), 2)
```

Loki - visitors to modify the IR

Transformer

- Traverses the IR and replaces nodes according to a given map
- Supports 1-to-many mappings (replace node with sequence)

SubstituteExpressions

- Traverses the IR and recurses into every expression tree
- Replaces expression tree nodes according to a given map

```
def remove_loops(routine, dimension):
    """
    Replace vector loops with their own bodies
    """
    loop_map = {}
    for loop in FindNodes(Loop).visit(routine.body):
        if loop.variable == dimension:
            loop_map[loop] = loop.body

    routine.body = Transformer(loop_map).visit(routine.body)
```

Loki - transformations

- Source code transformations can be defined using the `Transformation` class
  - `Transformation` class is the **building-block** in a transformation pipeline

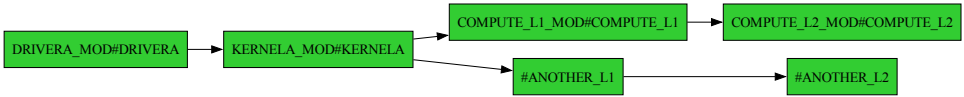
- Entry points at multiple levels:
  `transform_subroutine(), transform_module(), transform_file()`
- Can be applied to container data structures (`Sourcefile, Module, Subroutine`):
  ```
  MyTransformation().apply(sourcefile)
  MyTransformation().apply(module)
  MyTransformation().apply(kernel)
  ```
- `apply()` automatically dispatches to the relevant entry point level

Loki - bulk processing source trees

[WARNING] Scheduler is undergoing an incremental re-write!

- `Scheduler` applies transformations in bulk over call-trees

```
# Dependency tree for projA:
# projA: driverA -> kernelA -> compute_l1 -> compute_l2
#                        |
#                        | --> another_l1 -> another_l2
...
### define scheduler config via dictionary or config file
>>> config = {...}
>>> from loki import Scheduler
>>> scheduler = Scheduler(paths='projA', includes='projA/include', config=config, seed_routines=['driverA'])
>>> scheduler.callgraph('callgraph_simple')
```



- `Scheduler.apply(transformation)` applies a transformation to all items in the dependency graph
  - Can be applied "forward" or "backward"

Loki - SCC: Single Column Coalesced

- SCC "family" of transformations used to port IFS physics to GPU

- The baseline SCC is a multi-step transformation pipeline:
  - Resolve associates, explicit vector notation, masked conditionals, etc.
  - Remove CPU-style vector loops over horizontal
  - Demote array variables where possible
  - Re-insert horizontal vector loops around kernel
  - Insert OpenACC / OpenMP pragmas as appropriate

- Further (optional) transformations to reduce temporary array allocations on device:
  - Loki-SCC-hoist: Hoist temporaries to drivers
  - Loki-SCC-stack: Inject pool allocator with pre-computed stack size

- SCC transformations rely on certain coding norms
  - Remember, Loki is not a DSL ;)

Loki - SCC: single column formatting rules

- SC1: horizontal indexing
  - Variables referring to horizontal indices should be named consistently e.g. `JL`
- SC2: horizontal looping
  - All loops over the innermost, horizontal array dimension should be explicit (explicit array notation also ok)
- SC3: function calls from inside horizontal loops
  - Inside tight horizontal loops of type `DO JL=KIDIA,KFDIA` calls should be restricted to intrinsics
- SC4: no horizontal indirection
  - Indirect addressing on the innermost, horizontal array index shall not be used.
- SC5: no horizontal reduction across vector loop
  - No reduction operations (reducing the elements of an array into a single value) across the vector loop index `JL`
  - Although this introduces a horizontal dependency and is thus strictly speaking a violation of single column rules, Loki has functionality to facilitate this if needed
- SC6: no horizontal index array accessing with an offset
  - Arrays accessed in the horizontal dimension via the horizontal index should be accessed without any offset like e.g. `JL + n`

Loki - **loki-lint.py**

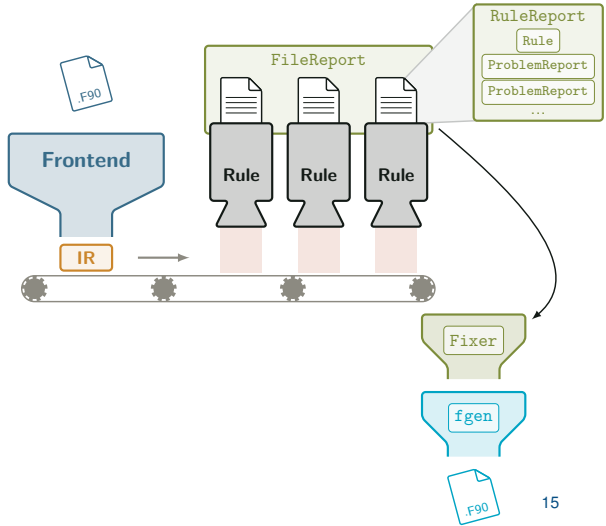
loki-lint.py: CLI tool to check code-base or call-tree against a configurable set of rules

CI code checking/linting

- **loki-lint.py** is run as part of the IFS CI suite

Interprocedural debugging utilities

- Argument intent linter: verify the correctness of subroutine dummy argument intent
- Argument size mismatch linter: check for size mismatch errors between arguments and dummy arguments



Loki - open development on github

- **Source code repository** on github: `https://github.com/ecmwf-ifs/loki`
- **Documentation** and install instructions: `https://sites.ecmwf.int/docs/loki/`
- **Bug tracking** and feature wish list: `https://github.com/ecmwf-ifs/loki/issues`
- **Tutorial** Jupyter notebooks: `https://github.com/ecmwf-ifs/loki/tree/main/example`
- **CLOUDSC** with multiple Loki transformations: `https://github.com/ecmwf-ifs/dwarf-p-cloudsc`

Thank you! Any questions?

References

1. Science and Technology Facilities Council. *fparser.* https://github.com/stfc/fparser.
2. Klöckner, A. & Contributors. *Pymbolic.* https://github.com/inducer/pymbolic.

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