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# Poseidon: A Source-to-Source Translator for Holistic HPC Optimizations of Ocean Models on Regular Grids

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## Main objectives of Poseidon

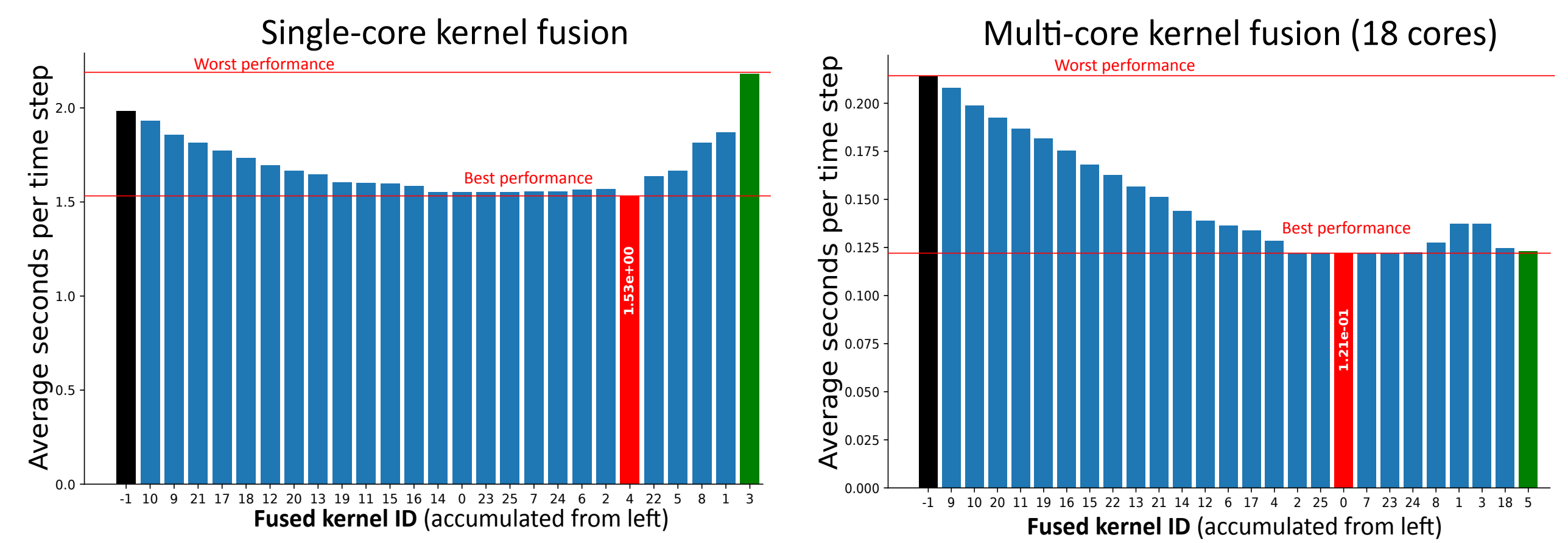
- Utilization of **existing Fortran code** (the main asset).
- Numerics experts can still write numerics code in Fortran **without hand-written HPC optimization**.
- Develop **method to automatically analyze, optimize and parallelize** such numerics code.
- Output is **source code** which is **compatible to existing ocean models** including used parallel programming models.
- First goal: **Models with regular grid structure**

## Abstract

- Ocean simulation** models play a **crucial role** in weather forecasts and **climate** change simulations.
  - However, they are often **far from the top performance** of computer architectures due to legacy programming styles.
  - Often, **entire codes are rewritten** which is often **too costly, time-consuming and error prone**.
  - In addition, **highly performing ocean models** require a **co-design**, including **MPI, automatic differentiation**, and many other features.
- This raises the research question "Whether it is possible to **translate existing Fortran code to reach top performance without rewriting of the entire code?**" motivating "Poseidon".

## Preliminary kernel fusion results

PDE model: **2D nonlinear barotropic solver** using an AB3/AM4 multi-step time integration scheme with all hand-optimizations undone.  
**Experiment:** Naive autotuning of kernel fusions using Poseidon, see below.  
**Hardware:** Intel® Xeon® W-2295 CPU @ 3.00GHz. / **Compiler:** nvfortran version 24.5-1.  
**Scalability:** Single-core and multi-core with OpenMP directives on 18 cores, without MPI, single CPU.  
**Correctness:** Tested against output of original source code.



### Kernel fusion by autotuning:

- Each "Fused kernel ID" is based on a kernel fusing all kernels of ID from left to this kernel ID. E.g., in left image, "21" refers to fusing kernels 10, then 9 and finally 21. No fusion is denoted by "-1".
- Selection of next kernel ID to fuse based on **steepest descent offline autotuning**.
- The last bar on the right shows the results of a **fusion of all possible kernels**.

### Discussion of results:

- Single-core vs. multi-core kernel fusion: **Kernel fusion provides higher speedups on multi-core systems** due to effects of roofline model.
- Speedup of x12 reached between the **best version on 1 core** (left graph) versus **best version on 18 cores** (right graph).
- Speedup of x16 reached between fully fused single core run (left graph) and best multi-core fusion.

## Overview of the Poseidon approach

### Stage 1: Input - PDE solvers written in Fortran

**Input:** Long-term goal is the application to the Nucleus for European Modelling of the Ocean (NEMO) [1], Coastal and Regional Ocean Community Ocean (CROCO) [2] model and to other developments (e.g., Flash-X).

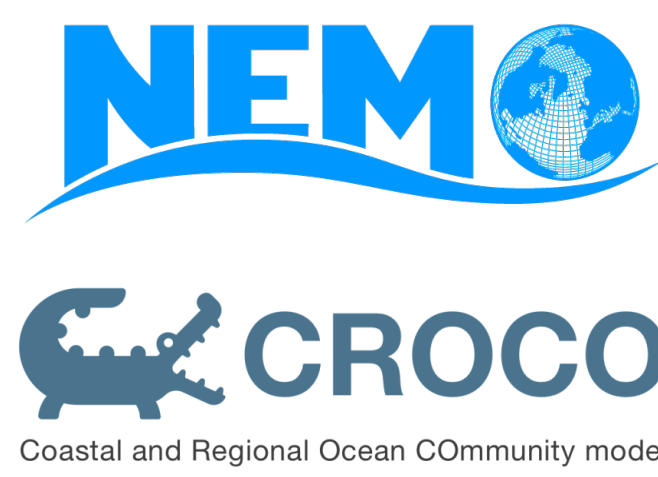
**Case study:** Research code using the numerics of the barotropic solver of the CROCO model  
**Example:** Multi-step extrapolation and computation of total height (in Croco model)

```

do j = jmin, jmax
  do i = imin, imax
    Drhs(i,j) = cff1 * zeta(i,j,kstp) &
               + cff2 * zeta(i,j,kbak) &
               + cff3 * zeta(i,j,kold) &
               + h(i,j)
  end do
end do

```

$$\zeta^{m+\frac{1}{2}} = \left(\frac{3}{2} + \beta\right)\zeta^m - \left(\frac{1}{2} + 2\beta\right)\zeta^{m-1} + \beta\zeta^{m-2}$$

$$D^{m+\frac{1}{2}} = \zeta^{m+\frac{1}{2}} + h$$


### Stage 2: Uplift through a PDE model-specific connector

We **extract** variables, computations, and their semantics with a model-specific connector based on PSyclone [3]. After this step, **all relevant information** is known about every variable and every access in the dynamical core.

#### 2.a Variables scope:

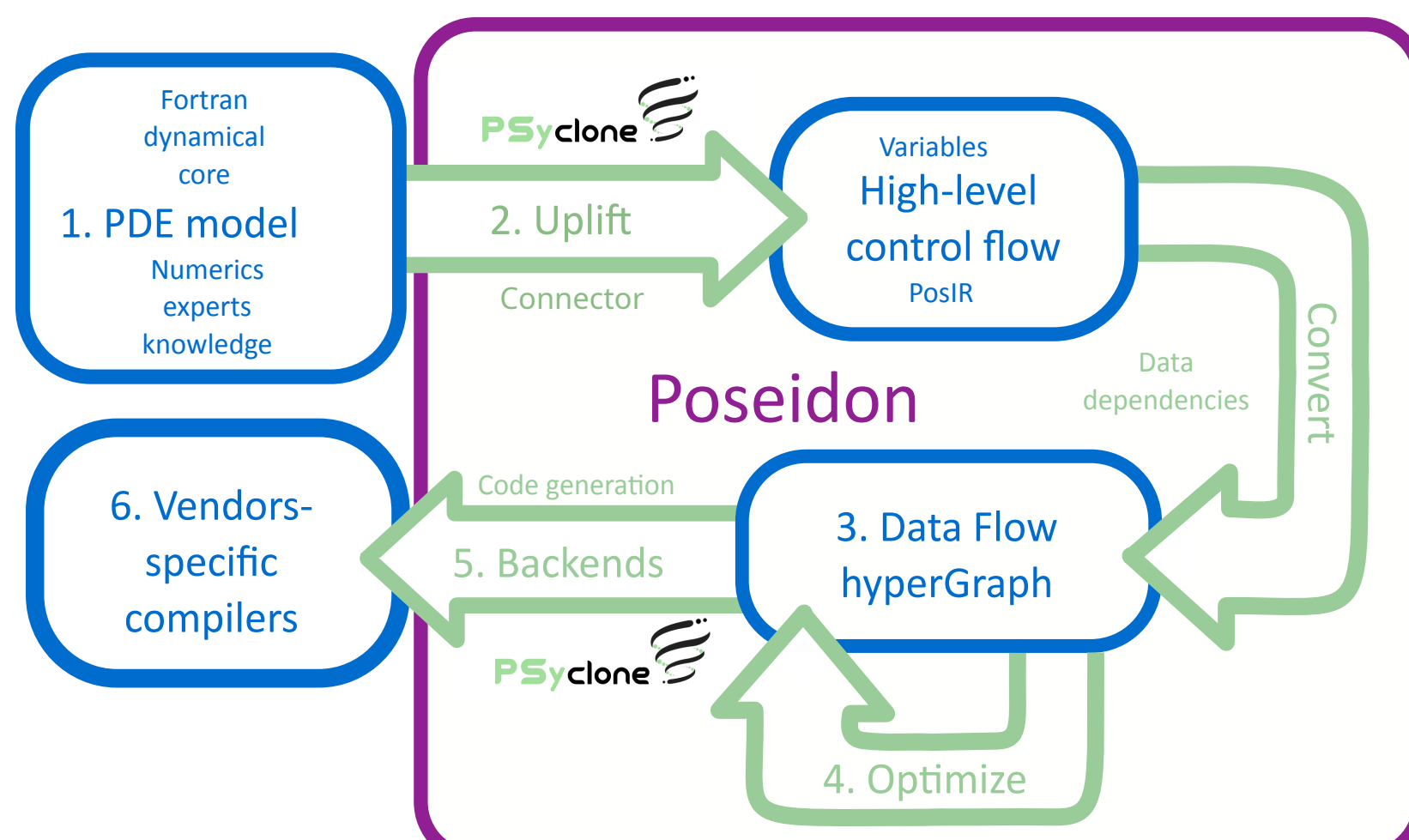
**High-level information** and meta data about **all variables** inferred from the code with the **PDE model-specific uplifter**.

**2.b Control Flow:** Nodes of the following types with a closure describing their input and output data dependencies. Based again on PDE model-specific uplifter.

- Kernel Loops:** DIM **nested loops** performing **stencil-like** operations, based on **PosIR**
- Boundary Conditions:** (DIM-1) **nested loops on boundaries**, with conditions, based on **PosIR**
- Computations:** All other computations, e.g., precomputed friction coefficients, based on **PosIR**
- Communications:** High-level abstraction of distributed communication
- Black Boxes:** Anything we do not yet support but can extract the closure from (I/O, printing, calls)

**Poseidon Intermediate Representation (PosIR):**

- List of assignment operations
- Assignment = numerical expressions
- Stencil-oriented
- Branches expressed as conditions



### Stage 3: Convert to a Data Flow Graph

- Convert to a **data flow graph** (see image to the right) with **hyperedges** between nodes representing **data flow**.
- This results in a **high-level intermediate representation** for further **graph-based operations** applicable in a **safe way**.

### Stage 4: Graph-based operations

- E.g. on kernel loops:
- Loop **splitting**
  - Kernel **fusion**
- Works in progress:
- Automatic **differentiation**
  - Injection of **communications**

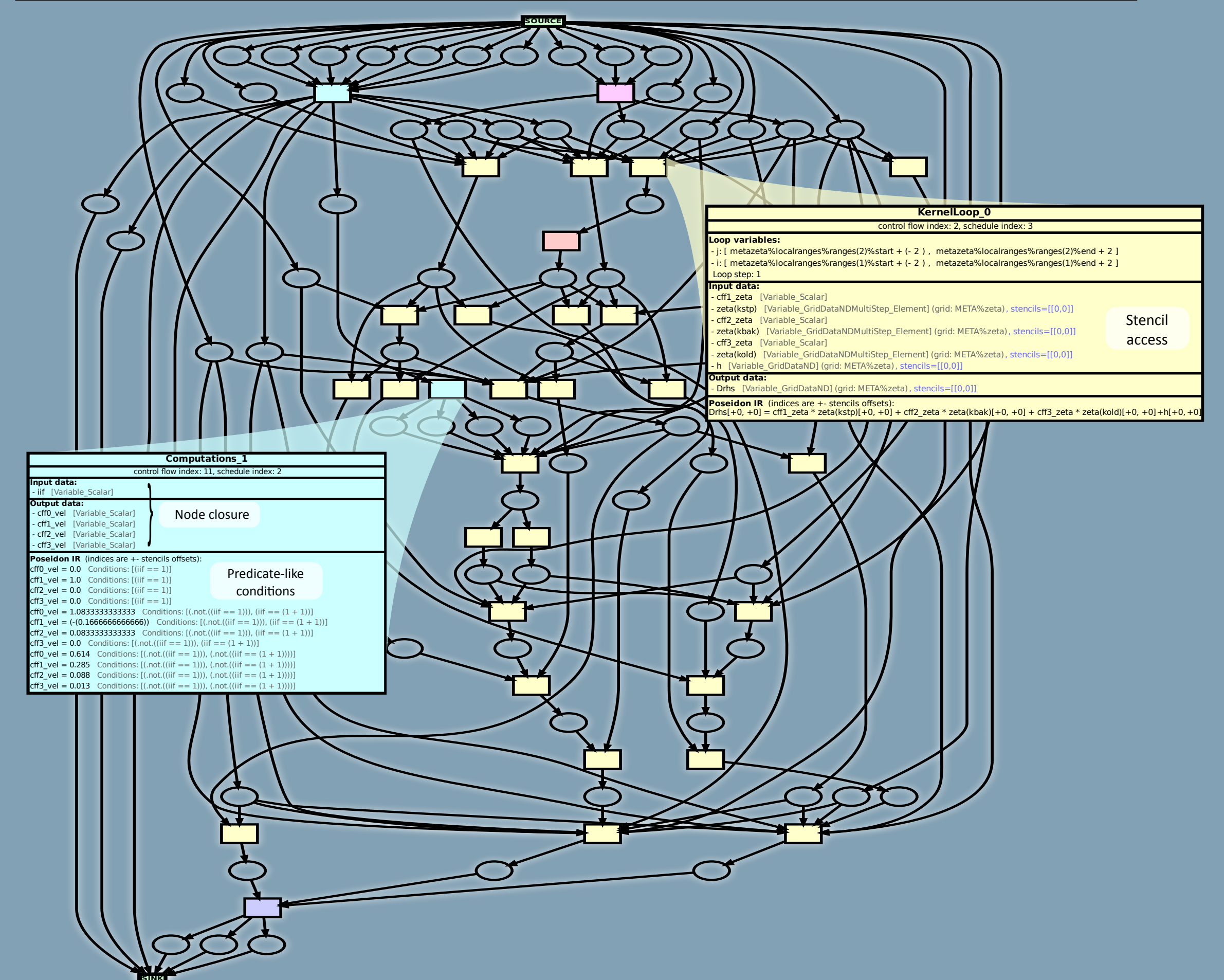
### Stage 6: Leverage vendors-specific compilers

- Poseidon is **independent of a specific compiler** as the next step in the compilation chain.
- Consequently, Poseidon can **leverage further optimizations** as performed by existing low-level and eventually hardware-specific compilers and communication backends.

### Stage 5: Code generation backends

- Create code for PDE model
- Pure Fortran with **PSyclone**
  - Parallel programming models for now: OpenMP, optional offloading to GPU
- Future work: Other parallel prog. models, IRs and DSLs

### Example of data flow hypergraph: Uplifted from a non-linear 2D barotropic multi-stepping solver with two of its Poseidon IR high-level nodes detailed.



## Poseidon limitations

### Uplifting:

- Requires to be **adapted to each model** (but Poseidon is python3 code, easy to get involved).
- Requires **correct extraction** of the numerics and control flow.

### Reliability:

- Failure of correct uplifting can lead to wrong results.
- 60% of the code is currently covered with unit tests (pytest).
- Continuous integration tests on 2 research code mini-applications.

## Summary

- Poseidon:** A new uplifting approach to a data-flow-oriented intermediate representation.
- Target:** **Holistic HPC optimization** of PDE models on regular grids written in Fortran.
- Avoids**
  - hand-tuned codes** (making code often less understandable),
  - entire rewrites of code** in another domain-specific language (often not accepted by numerics experts),
  - introducing errors in numerics** by rewriting code, e.g., in new domain-specific language
- Approach:** Uplifting brings back the semantics of the numerical model through PDE model-specific connectors. Further steps allow performance optimizations on data flow graph.
- Retains the original Fortran code** which is considered to be a **highly-valuable asset**.

## Future research directions

### Near-term goals:

- Developing uplifting connectors to **production codes**, including NEMO ocean model.
- Reduce arithmetic intensity** by simplifying kernel numerics after kernel fusion.
- Implementing **more graph operations**, e.g., array buffer reuse and loop fusion.
- Automatic **distributed-memory communication** and **latency hiding strategies**.
- Automatic differentiation** of data flow graph followed by graph-based optimization.

### Long-term goals:

- Support other **programming models** (OpenCL, OpenACC, etc.) and **hardware** (e.g., FPGAs)
- Extension to **unstructured grids**

## Related work

Usage of DaCE [5] to optimize FV3, an Earth System Model, originally written in Fortran. Optimizations are similar to those aimed with Poseidon, but the PDE solver has been entirely rewritten in Python3.

PSyclone [3] is a source-to-source Fortran compiler written in Python. It allows us to easily parse Fortran code and create our own Intermediate Representation based on a Data Flow Graph in Poseidon.

In [4] Nick Brown et al. present an extension of the Flang LLVM MLIR Compiler to extract stencil patterns from Fortran source code. Writing their framework as a compiler pass, they are able to leverage existing MLIR dialects and transformations. Contrary to this approach, e.g., our source-to-source code transformation framework allows us to use any general purpose compiler.

## References

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