HPC Programming for the Future

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Caveats

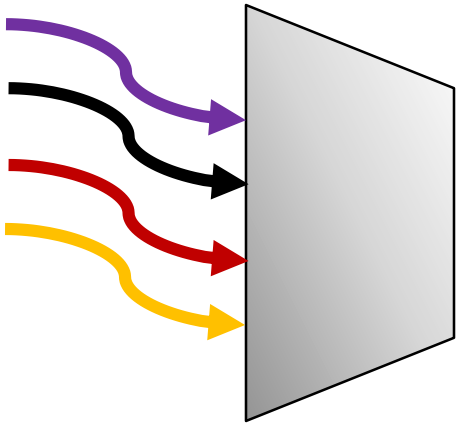
- **This is a forward-looking, what-if presentation**
- **Should not be taken as conveying our product plans**

- **I'm wearing my broader-community hat, not my speaking-for-Intel hat**

Outline

- Some challenges
- Language interfaces
- OpenMP
- Data layout
- Library directions

Building a community



Share problems

Explore, vet, implement

Converge on standards

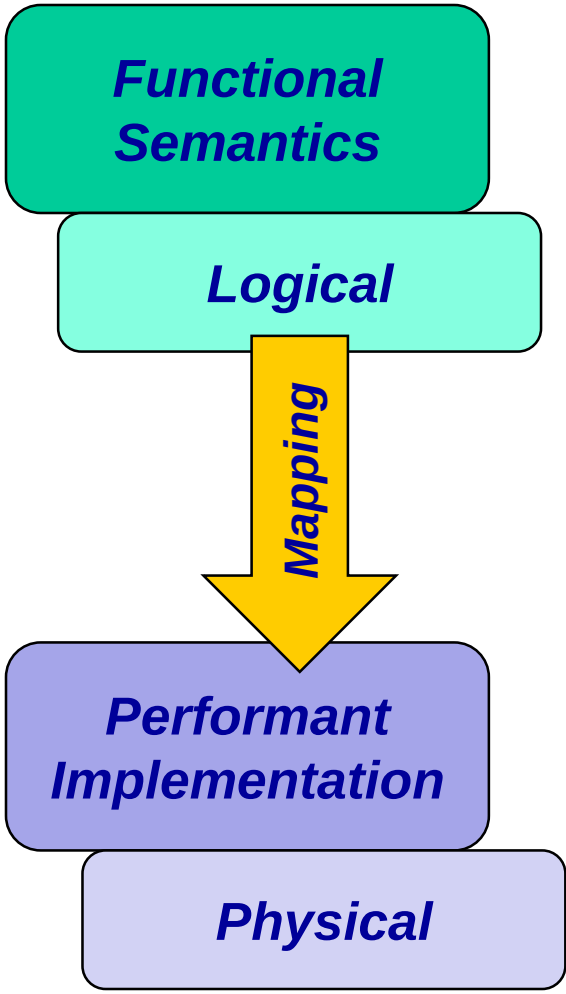
Some challenges

- **Exposing parallelism**
  - Language interfaces
  - Future proofing
- **Controlling how parallelism is harvested**
  - Concurrency
  - Distribution
  - Data layout

- ***See padalworkshop.org for forthcoming report out to broader HPC community***

Layering

- **Semantic layer**
  - Describe the "what"
  - Expressiveness, intuitiveness, productivity
  - Minimalist
- **Performance control layer**
  - Describe the "how"
  - Control, efficiency
  - More pervasive
  - Achieve re-targetability through encapsulation
- **Separation of concerns**
  - Domain expert ≠ tuning expert
  - Different objectives, different rates of change, different lifetimes



Language interfaces

- **Semantic layer**
  - Less content, but it's more stable
  - More standard, but standards change more slowly
  - Influence languages, like **C++**
  - Use directives that are backed by compiler support and runtime libraries, like **OpenMP**
  - Use functional libraries, like **MKL, NumPy**
- **Performance control layer**
  - More things to control → more content
  - More innovation → harder to standardize
  - Influence and develop libraries, which can change faster than compilers, like **OpenMP, Kokkos**

OpenMP

- **Strengths**
  - Standard, widespread, natural
  - Spans semantic and control layers
- **Weaknesses are redeemable**
  - Composability issues
  - Has some holes in its completeness
- **Transitions (see below for "→")**
  - Improved compiler support for outer-loop parallelization
  - Offload is synchronous only → async
  - Data must be structured → decoupled from control structures
  - Constrained by C++ rules to not pass structs as parameters →
  - Each nesting layer thinks it owns the whole machine →
  - [Usage] Each library call manages OpenMP independently →

Semantic layer: expose

- **Map serial specification of work onto parallel data collections**
  - What to do should be separable from the order in which it's done
  - Ex: OpenMP simd functions, lambda functions, Kokkos
  - Enrich this appropriately, e.g. with reductions, compress/expand
- **Specify data reference patterns**
  - Pass domain-expert knowledge to underlying system
  - Mix of reads and writes: read-only, write-once, mixed
  - Spatial locality: streaming, strided?, random
  - Temporal locality: use once, reused, persisted
  - Other: high bandwidth, working set size, etc.

Performance control layer: harvest

- **Support for parallelism**
  - SIMD/vector
  - Threads in a core
  - Cores in a node
  - Nodes in a cluster
- **Temporal**
  - Dimension order
  - Blocking
  - Work stealing
- **Binding and data layout**
  - AoS, SoA, AoSoA, …
  - On package or not
  - Shared or distributed

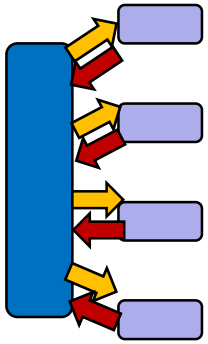
Data layout challenges

- **Use of structs**
  - C++ template-based abstractions like Arrow Street, SIMD Building Blocks, maybe supported by extensions for reflection/introspection
- **Best traversal of multi-dimensional arrays**
  - Inner vs. outer loop level – directing parallelization
  - Blocking – directing traversal via insertion of nests
  - Spanning multiple access patterns – selective data re-layout
  - Abstract functions + target-tuned traversal libraries
- **Discerning access patterns**
  - Assumed-shape and pointer arrays: stride 1 or not?
  - Temporary arrays
  - MACVEC tool at TACC – LCPC submission with Jim Browne *et al*
  - Forthcoming Advisor/Vector Tool from Intel moving in this direction

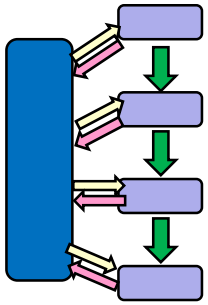
Library directions for expansion

- **Distributed**
  - Homogeneous cluster
  - Heterogeneous cluster
  - libhta
- **Grey-box vs. black-box libraries**
  - Inlinable specialization with static guidance by users
  - Multi-phase
  - Persist distributed data
  - Decouple naming of parameters from their availability
  - OpenFOAM collaboration with Doug James
  - Parallel regions defined outside of library calls vs. within them
- **Specialized**
  - Branching in inlinable header files – error checking, special casing
  - Special sizes and shapes, with adequate motivation

"Grey-box libraries"



- **Current way**
  - All inputs are in one place
  - Call library, which returns all outputs
  - Rinse, repeat
- **In contrast**
  - Initialize: distribute, (re-)format (SpMV)
  - Execute: sequence or iterate
    - Mix of stable variables and updates
    - Inputs and outputs may be distributed
    - Overlap computes and communication
    - Each partition works on its own portion



Remember…

- **This is a what-if presentation, not a roadmap**
- **Comments on other discussions**
  - 15.0 compiler has much better support for vectorization, including better support for outer loops, way better reporting
  - In 15.0, MKL headers that do error checking, specialization, and native compilation fallback in C
  - MPSS 3.3 enhanced to support MIC-MIC proxy transfers within a node, which significantly boosts bandwidth for multiple cards

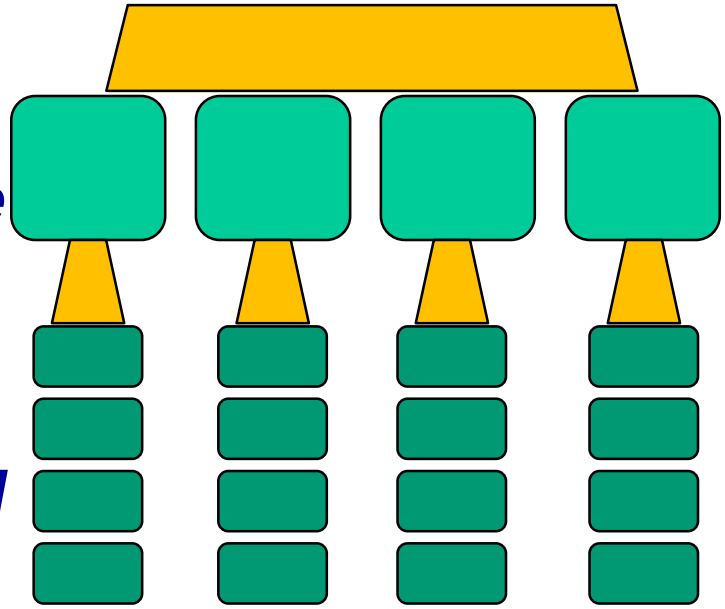
Backup

- **Structs as parameters**
  - See my talk at padalworkshop.org
- **OpenMP in a hierarchy**
- **Temporary array example**
  - Omitted pending permission
- **Challenges of abstraction**
- **Mapping scalar work to collections and targets**
- **How to specify properties**

The nested OpenMP problem

4-wide
Whole machine

Nested
Oversubscribed

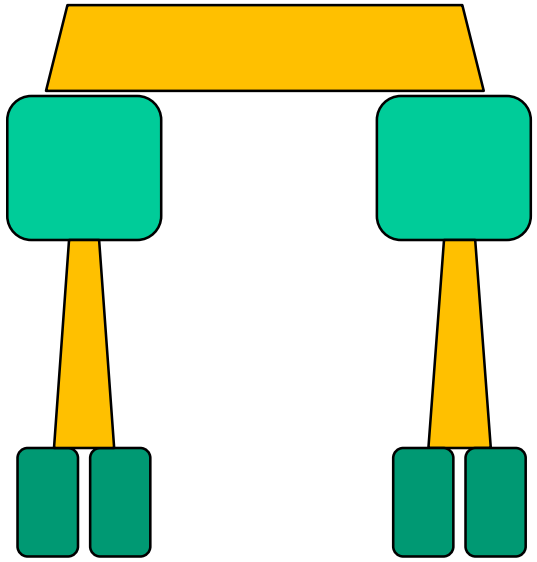


```
main() {
  omp parallel
  function()
  …
}

function() {
   omp parallel for
   …
}
```

- **Nested but context oblivious**
- **Each layer thinks it owns the world (e.g. 4 wide)**

Avoid OpenMP nesting with a hierarchy



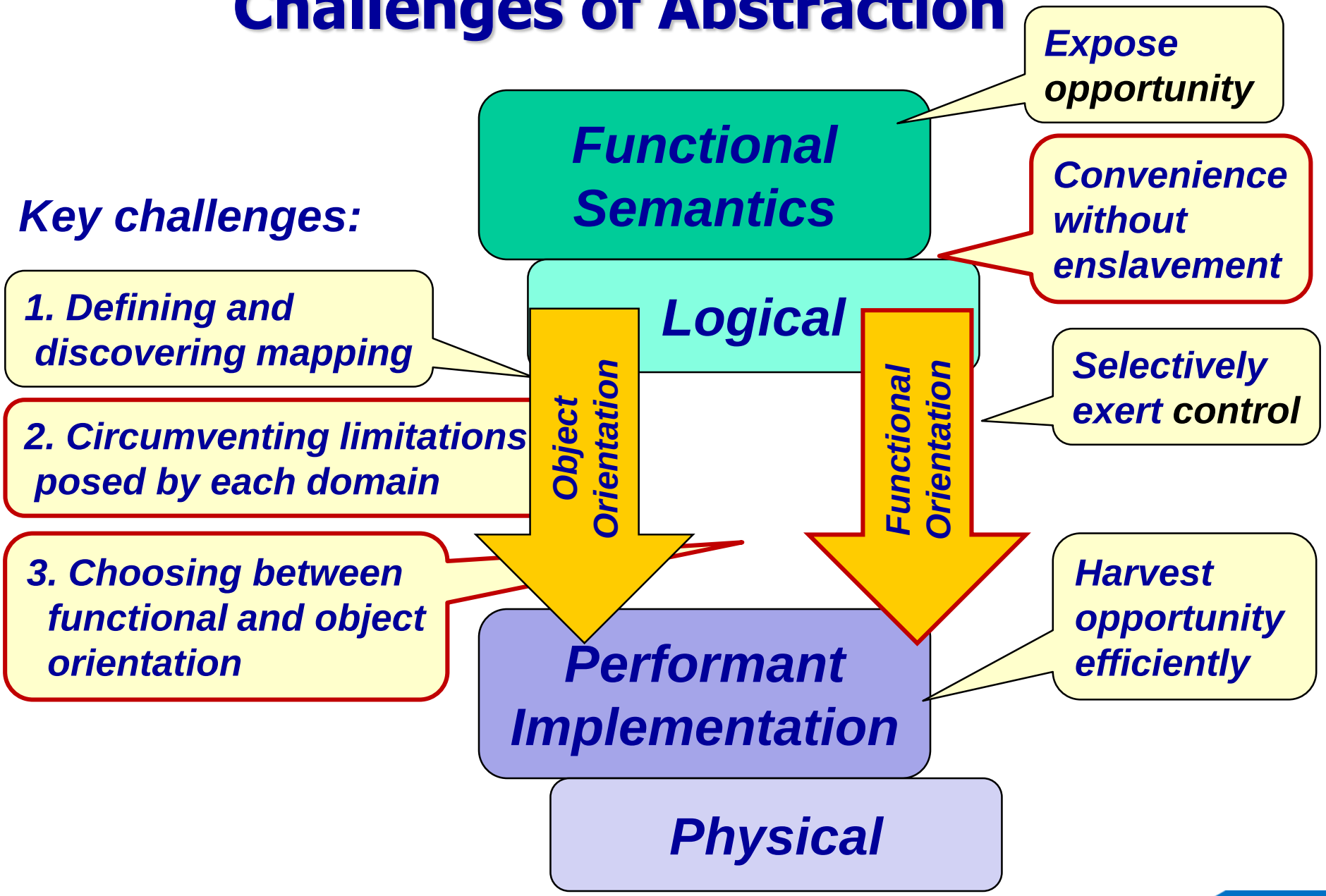
```
main() {
  establish_partitions(P)
  distribute_work(P)
  sync()
}

do_work(P) {
   omp parallel for
      work(P)
}

work(P) {
  i = omp_thread_num()
  // do ith part of P
```

- **OpenMP isn't what does the nesting**
- **Hierarchy established outside of OpenMP context**

Challenges of Abstraction



"Scalar" work → {collections, targets}

Scalar work

```
struct.x = f(…)
struct.y = g(…)
struct.z = h(…)
```

Support for parallelism

- SIMD/vector
- Threads in a core
- Cores in a node
- Nodes in a cluster
- …

Data collec-tions

- Multi-dim arrays
- Irregular
- Hierarchical …

Tem-poral

- Dimension order
- Blocking
- Work stealing …

Ref patterns

- Working set size
- Access pattern

Data layout

- Array of structs (AoS)
- Struct of arrays (SoA)
- AoSoA …

Binding

- On pkg or not
- Shared or distributed

- Separation of concerns
- Mapping problem
- Want flexibility through abstraction, + control

How to specify properties

	Property	Data type	Function modifier	Pragma on construct	Comments
Semantic property	Scalar work	-	-	-	Algorithmic freedom
	Data collection	√			*Kind* vs. organization
	Reference patterns	√	√	√	Size and logical patterns
Con-ven-ience	Logical data layout	√			Merge with data collection?
Performance property	Physical data layout	?	√	√	What's proximate in physical arrangement
	Temporal		?	√	Work order affects access patterns
	Supported parallelism	√	√	?	Want data to match compute
	Binding		√	√	Binding to places