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Flexible, Efficient Abstractions for High Performance Computation on Current and Emerging Architectures

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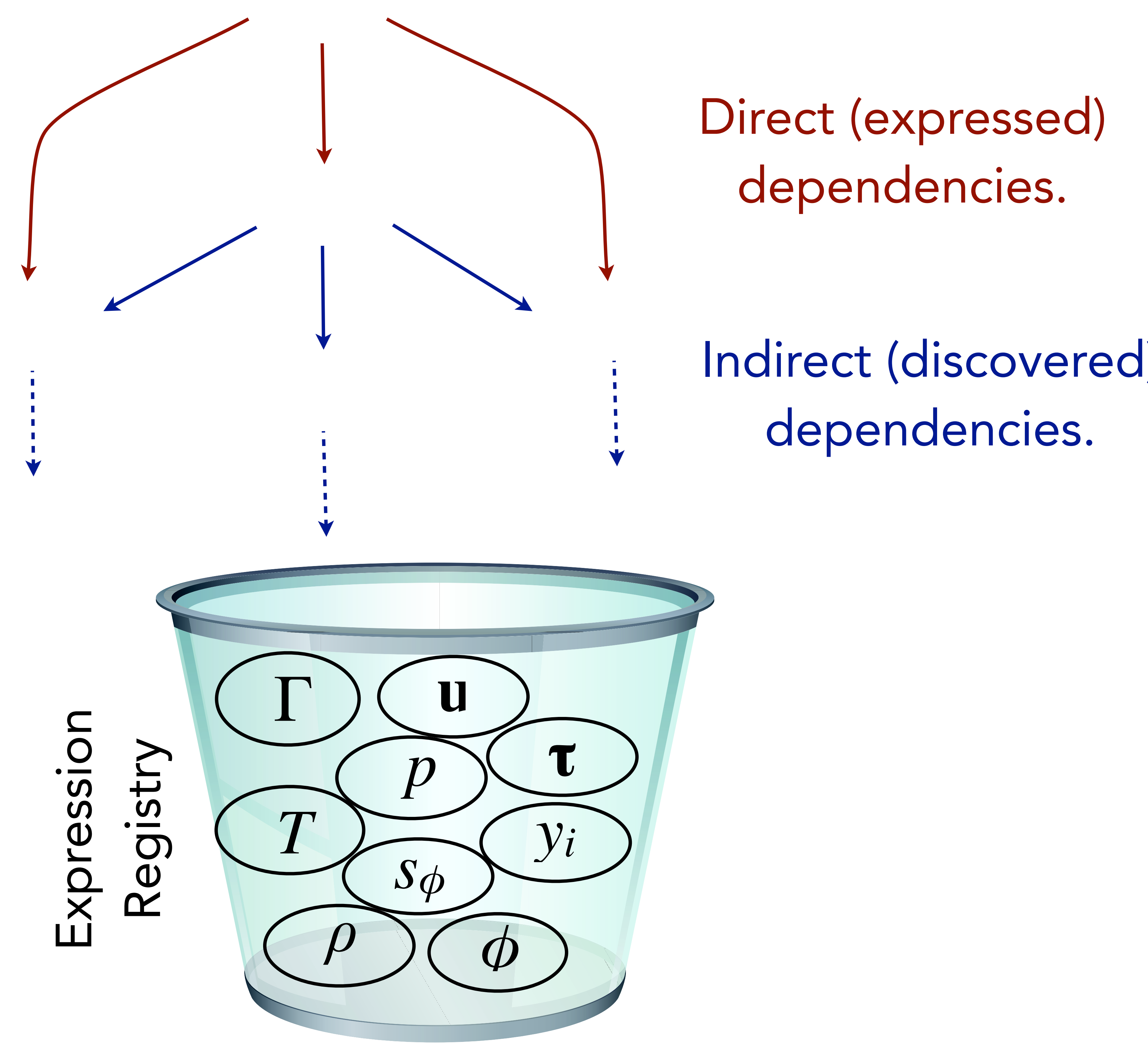
Motivation

- Complex physics ⇒ complex software!
  - *is this necessary, or just a result of looking at the problem in the wrong way?*
- Changing from model "A" to model "B" ...
  - *may require different transport equations*
  - *may introduce different nonlinear coupling*
- Spatial discretization frequently permeates software design
  - *Model developers typically must deal with "mesh loops"*
    - often resort to "copy/paste/modify" tactics that are highly bug-prone
  - *Future proofing:*
    - What if you want to do OpenMP on these loops?
    - What happens when you learn that OpenMP is not the right tool?
    - pthreads, CUDA / OpenCL ... ?
- Questions: Can we write efficient software that...
  - *... naturally handles complexity and allows us to easily extend/replace existing models?*
  - *... allows programmers to easily and robustly express intent while not worrying about "details?"*
  - *... allows us to refactor for different hardware architectures without rewriting the code base?*

Flexible…

- Register all expressions
  - *Each "expression" calculates one or more field quantities.*
  - *Each expression advertises its direct dependencies.*
- Set a "root" expression; construct a graph
  - *All dependencies are discovered/resolved automatically.*
  - *Highly localized influence of changes in models.*
  - *Not all expressions in the registry may be relevant/used.*
- From the graph:
  - *Deduce storage requirements & allocate memory (externally to each expression).*
  - *Automatically schedule evaluation, ensuring proper ordering.*
    - Asynchronous execution is critical! (overlap communication & computation)
  - *Robust scheduling algorithms are key.*

$$\Gamma = \Gamma(T, p, y_i)$$



*Notz, Pawlowski, & Sutherland (2012). ACM Transactions on Mathematical Software, 39(1).

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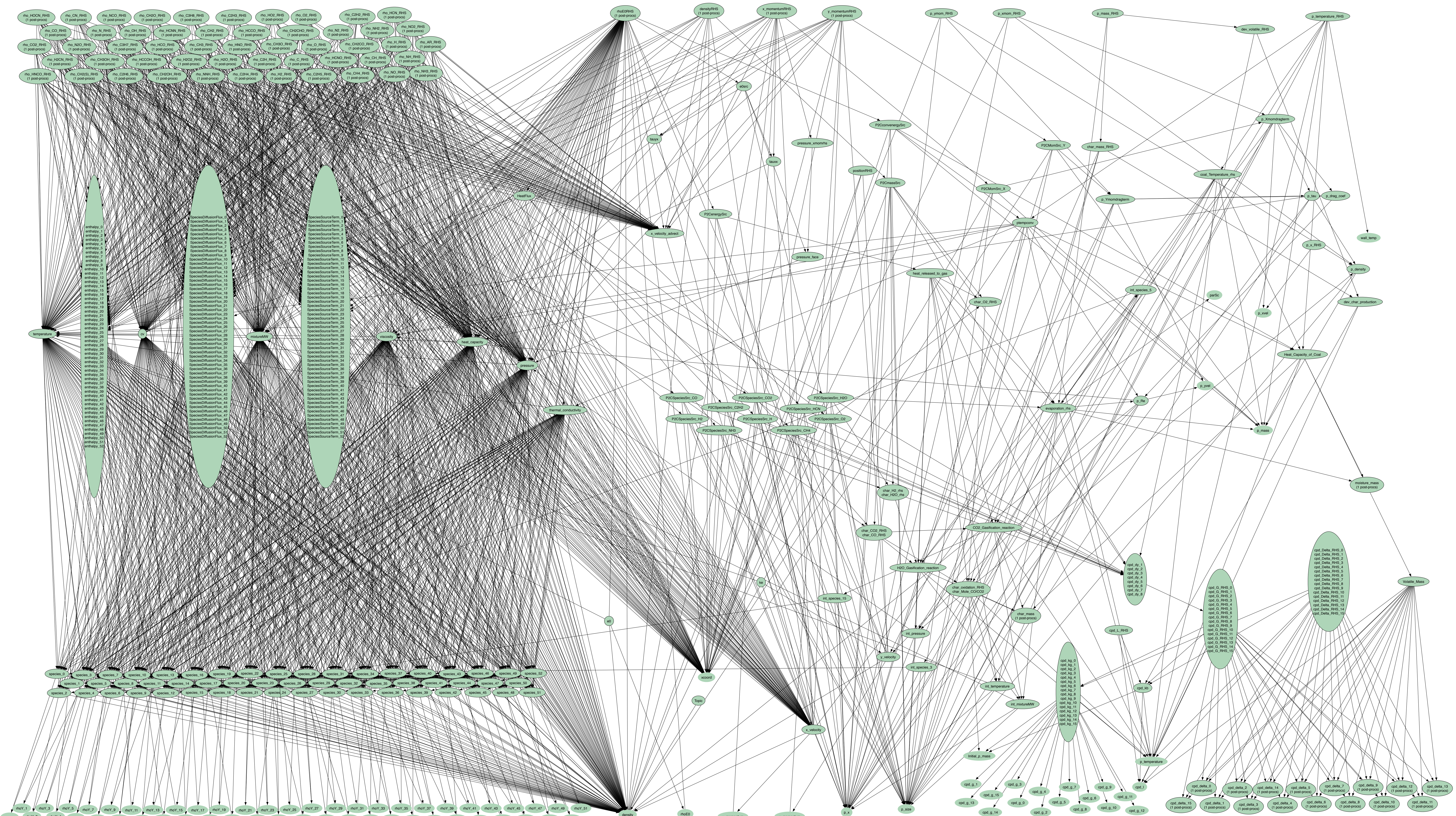
Example: coal combustion

- 55 PDEs
- ~35 ODEs per particle
- Complex interphase coupling



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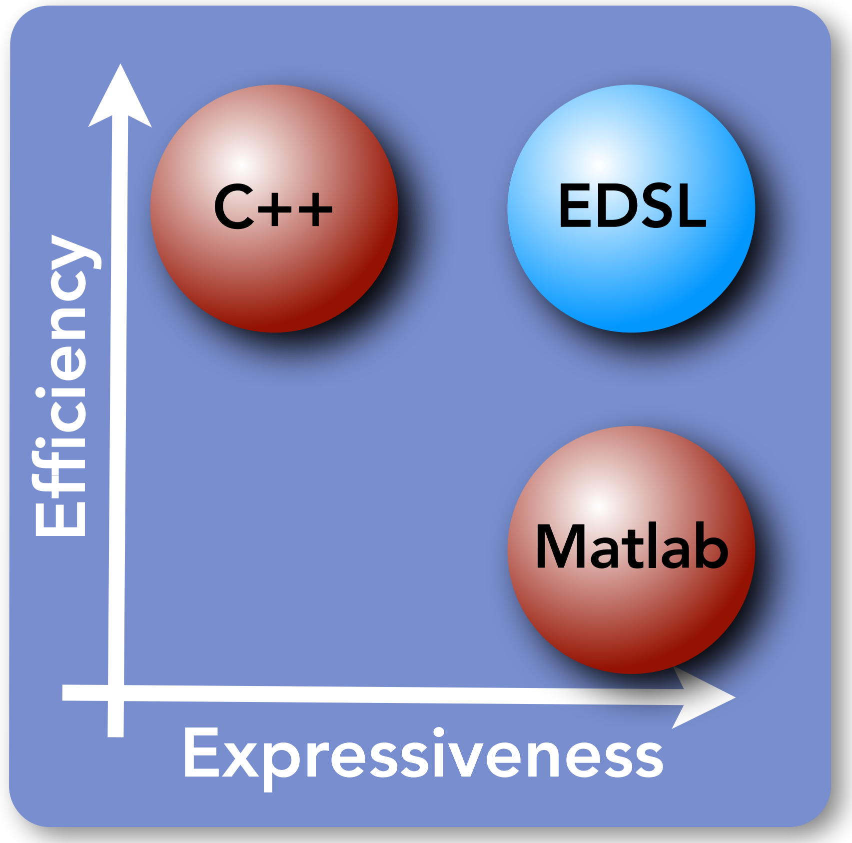
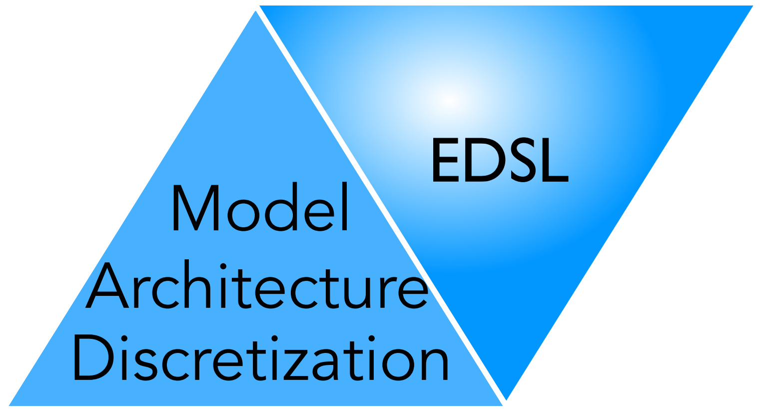
Efficient…

- Expressive syntax (matlab-style array operations)
  - *Programmer expresses intent (problem structure) - not implementation.*
- High performance
  - *Should match hand-tuned code in performance.*
- Extensible
  - *Insulate programmer from architecture changes (e.g. multicore → GPU → …).*
  - *EDSL "back-end" compiles into code for target architecture.*
- "Plays well with others"
  - *Allow programmer to write in C++ and inter-operate with EDSL.*
  - *Not an "all-or-none" approach: enable incremental adoption.*
  - *Allows concurrent development of EDSL and application codes.*





Field Expressions

$$\vec{c} = \vec{a} + sin(\vec{b})$$

Manual C++

Thread 1

```
Field::const_iterator ia1 = a1.begin();
Field::const_iterator ib1 = b1.begin();
for(Field::iterator ic1 = c1.begin();
    ic1 != c1.end();
    ++ic1, ++ia1, ++ib1) {
  *ic1 = *ia1 + sin(*ib1);
};
...
```

⋮

Thread n

```
Field::const_iterator ian = an.begin();
Field::const_iterator ibn = bn.begin();
for(Field::iterator icn = cn.begin();
    icn != cn.end();
    ++icn, ++ian, ++ibn) {
  *icn = *ian + sin(*ibn);
};
```

Nebo EDSL

```
c <<= a + sin(b);
```

- Data parallel handled internally.
- Thread deployment (resizable threadpool).
- GPU deployment.
- Compile-time guarantee of field compatibility for given operations.

Chained Stencil Operations

$$\phi = -\nabla \cdot \mathbf{q}$$
$$= \nabla \cdot (\lambda \nabla T)$$

```
phi <<= divX( interpX(lambda) * gradX(temperature) )
      + divY( interpY(lambda) * gradY(temperature) )
      + divZ( interpZ(lambda) * gradZ(temperature) );
```

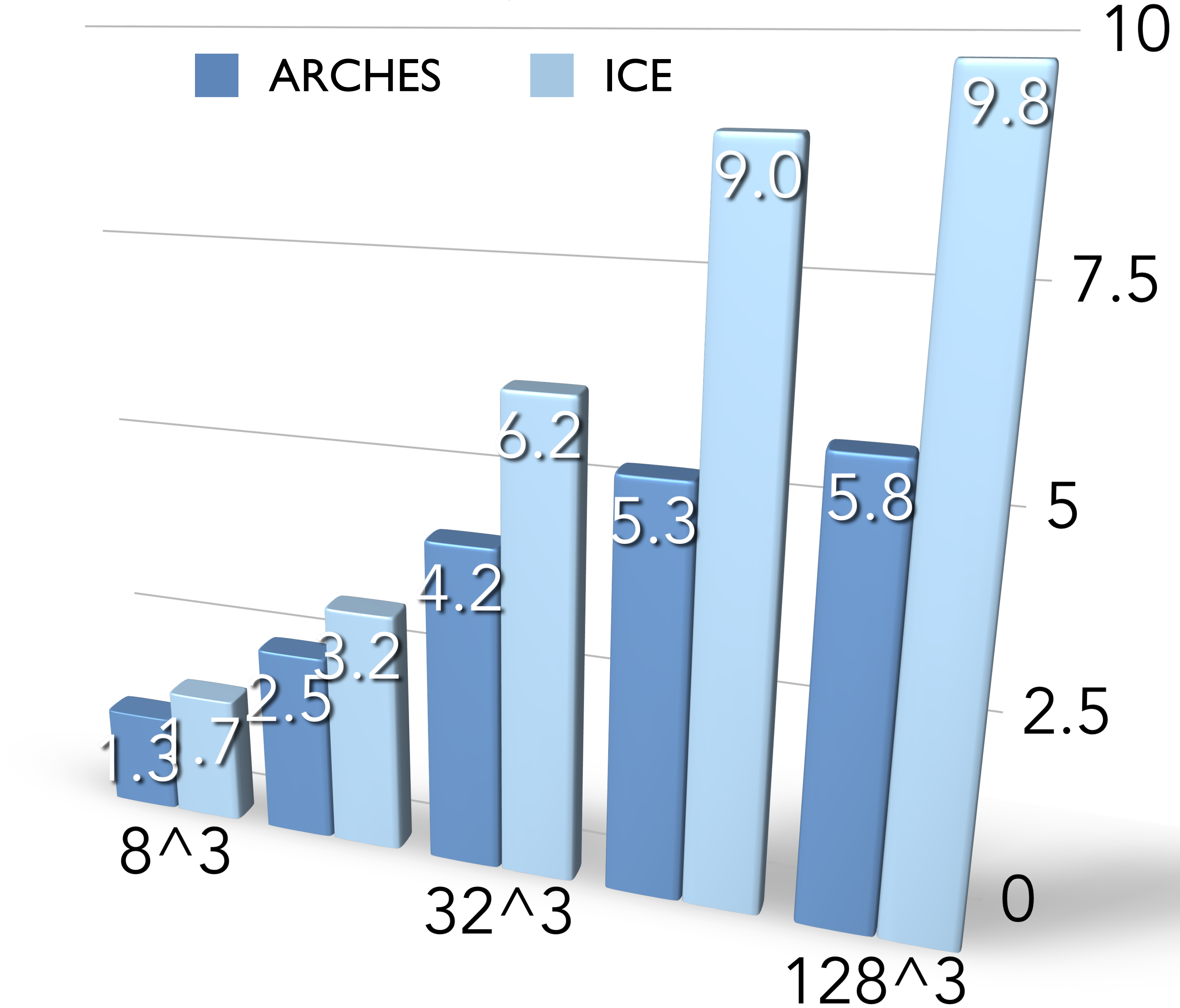
```
// field type inference:
typedef FaceTypes<FieldT>::XFace  XFluxT;
typedef FaceTypes<FieldT>::YFace  YFluxT;
typedef FaceTypes<FieldT>::ZFace  ZFluxT;

// operator type inference:
typedef OpTypes<FieldT>::DivX  DivX;
typedef OpTypes<FieldT>::DivY  DivY;
typedef OpTypes<FieldT>::DivZ  DivZ;
```

- One inlined grid loop, no temporaries.
- Better performance & scalability than without chaining.
- Compile-time consistency checking (field-operator and field-field compatibility).
- Runtime consistency checks for ghost cell validity.

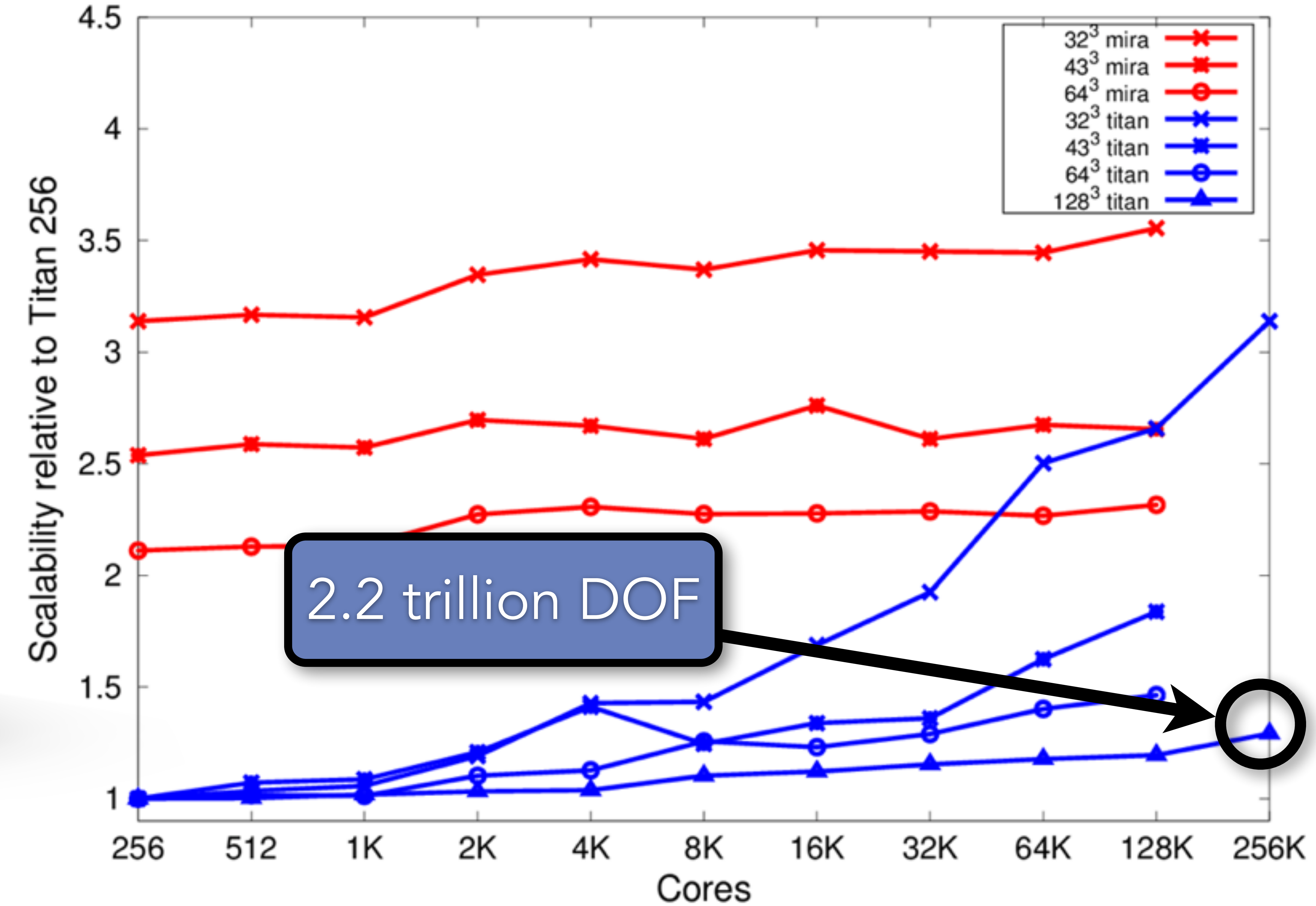
Putting it Together: Performance & Scalability

Speedup using DSL* relative to other Uintah codes



*Comparison to ICE and ARCHES, sister codes in Uintah, on a 3D Taylor-Green vortex problem. Run on a single processor.

Weak scaling on Titan



"1" indicates perfect weak scaling

Multicore & GPU Performance

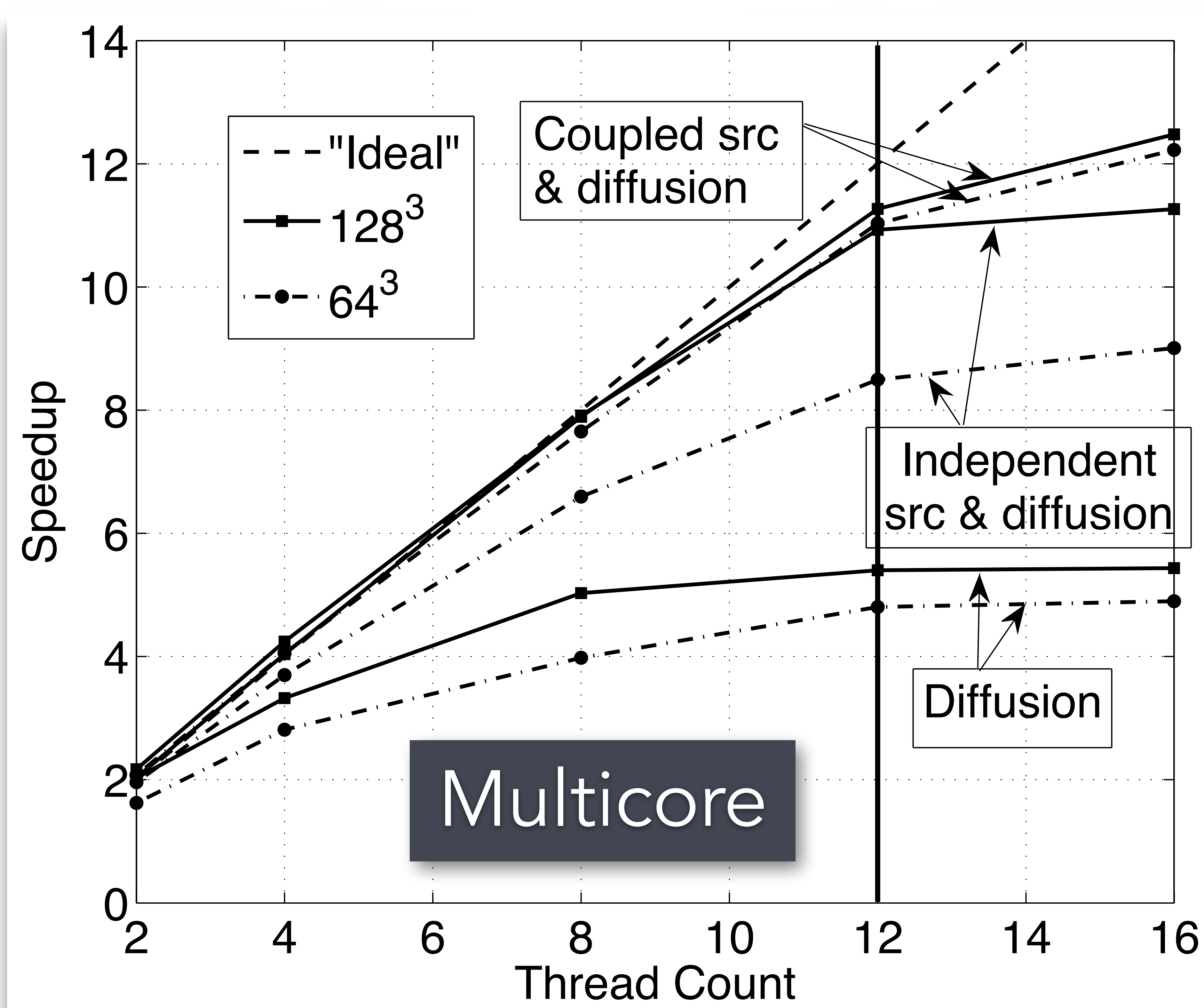
Test: mockup of a diffusion-reaction problem.

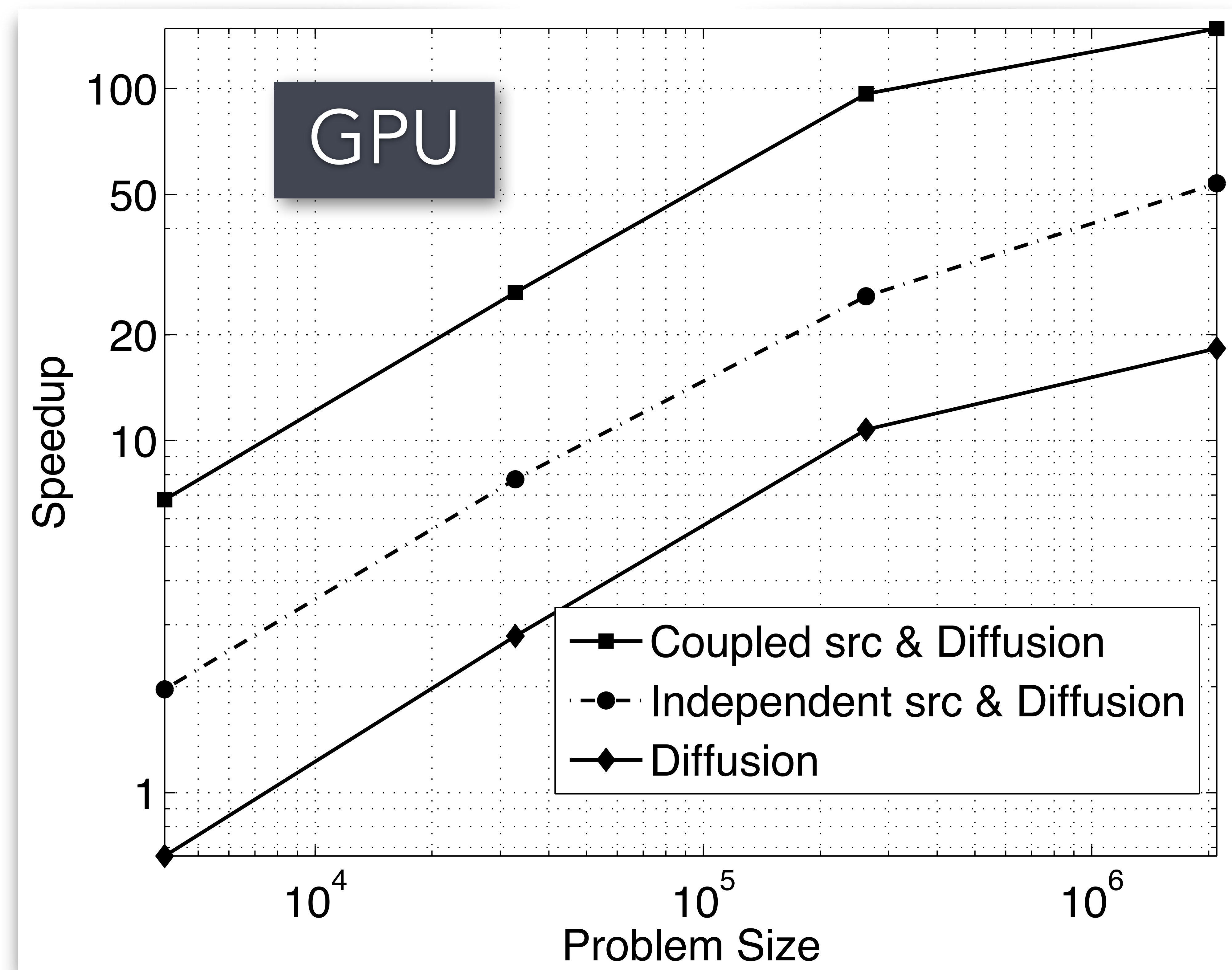
- Easily dial in the number of equations (30 here).
- Diffusion is an inexpensive stencil calculation.
- Reaction is an expensive point-wise calculation.

$$\frac{\partial \phi_i}{\partial t} = -\nabla \cdot \mathbf{J}_i + s_i$$

$$\mathbf{J}_i = -\Gamma \nabla \phi_i$$

$$s_i = f(\phi_i) \text{ or } s_i = f(\phi_j)$$





Parting Thoughts

- Hierarchical parallelization allows for flexible usage of available resources:
  - *Domain decomposition (SIMD)*
    - Should allow a process to do computation on "interior" while waiting on communication from neighbors.
  - *Task decomposition (MIMD)*
    - Decompose the solution into a DAG that can be scheduled asynchronously.
  - *Vectorized parallel (SIMD)*
    - Break grid operations across multicore, GPU, etc.
- DAG representation is a scalable abstraction that:
  - *Handles problem complexity gracefully.*
  - *Provides convenient separation of the problem's structure from the data.*
  - *Allows sophisticated scheduling algorithms to optimize scalability & performance.*
- (E)DSLs are very useful
  - *Future-proofing: separate intent from implementation.*
  - ***E**DSLs allow seamless transition of a code base and leverage existing compilers.*
  - *Template metaprogramming pushes work from run-time to compile-time for more efficiency.*

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