ICSE
THE INSTITUTE FOR CLEAN AND SECURE ENERGY
▪155 South 1452 East Room 380 ▪Salt Lake City, Utah 84112 ▪1-801-585-1233

Graph-Based Parallel Task Scheduling and Algorithm Generation for Multiphysics PDE Software

James C. Sutherland
ASSISTANT PROFESSOR - CHEMICAL ENGINEERING

Devin Robison
M.S. STUDENT

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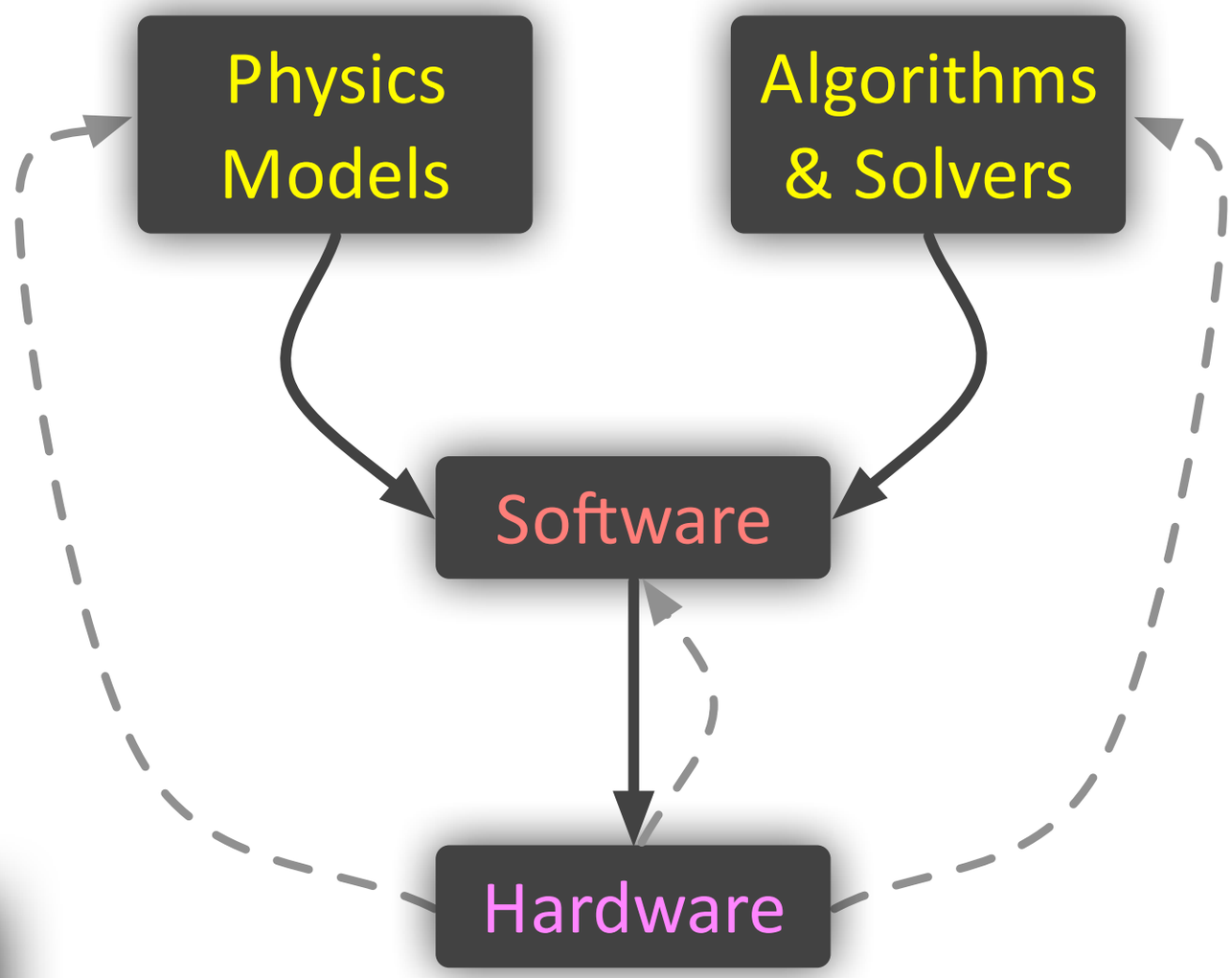
This work was funded in part by NSF PetaApps award 0904631
National Science Foundation WHERE DISCOVERIES BEGIN

Motivation

Physics is complex & changing

Software must handle complexity & changing nature of:

- physics models,
- algorithms,
- hardware

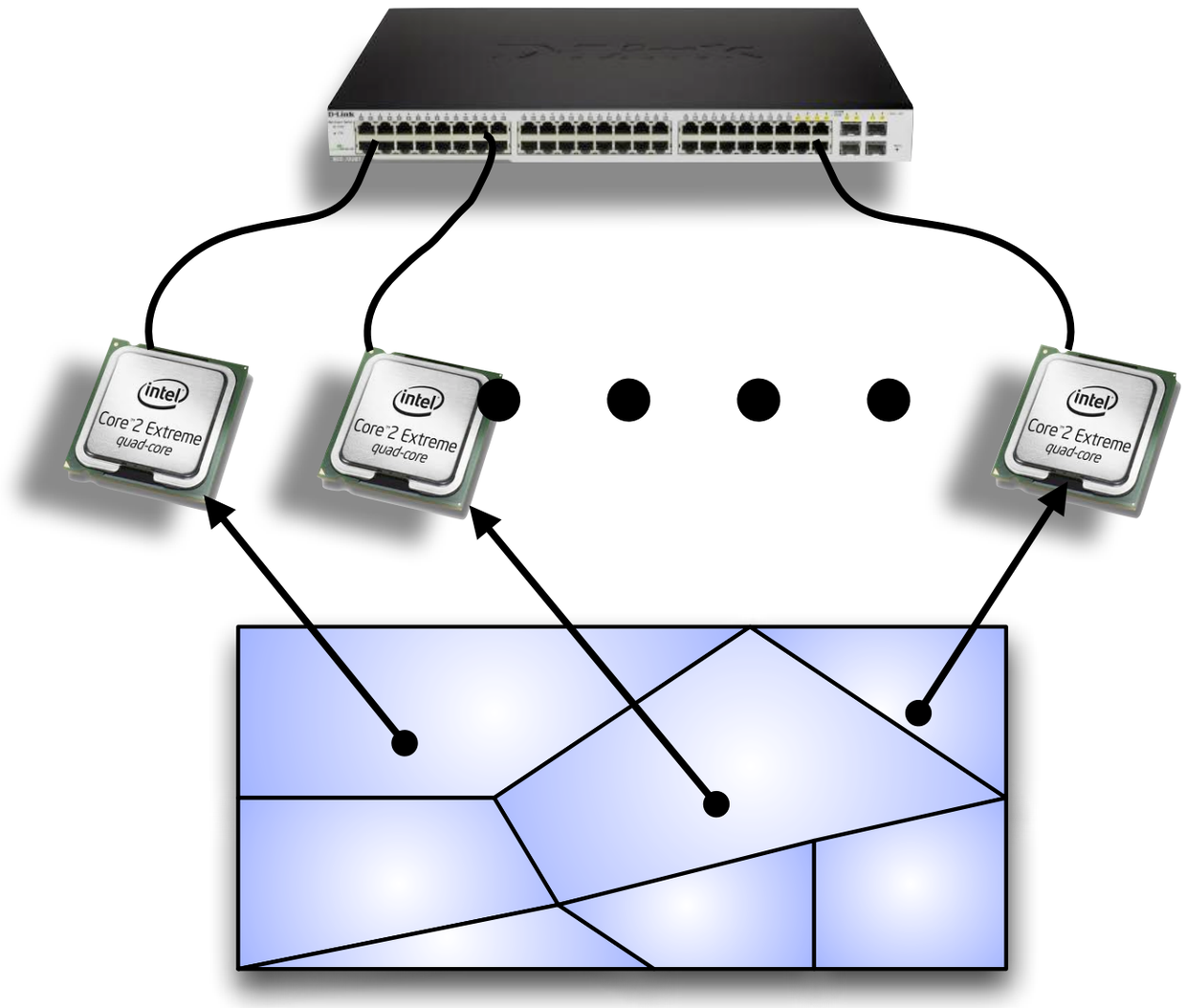


Hardware is complex & changing

- muticore/manycore
- hybrid CPU/GPU or other accelerators

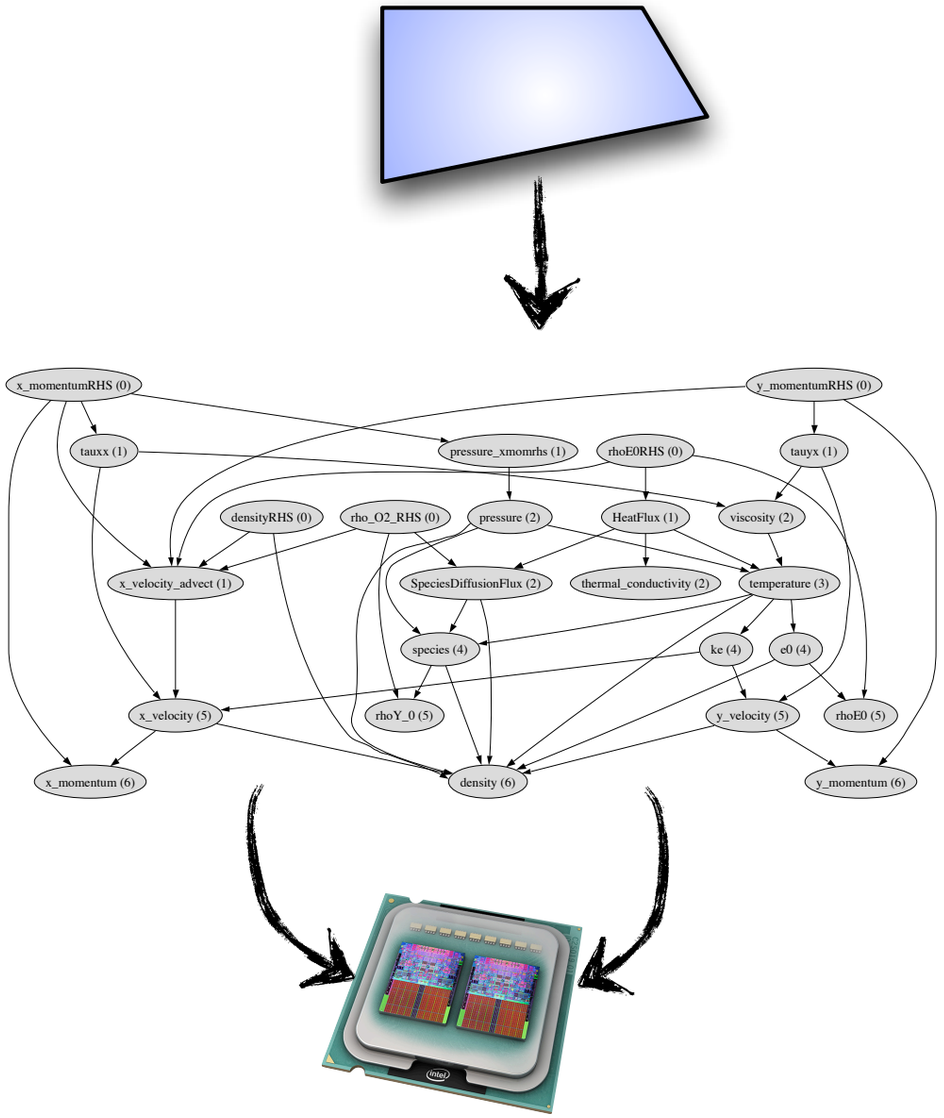
Hierarchical Parallelization

- Domain decomposition
  - data parallel (MPI)



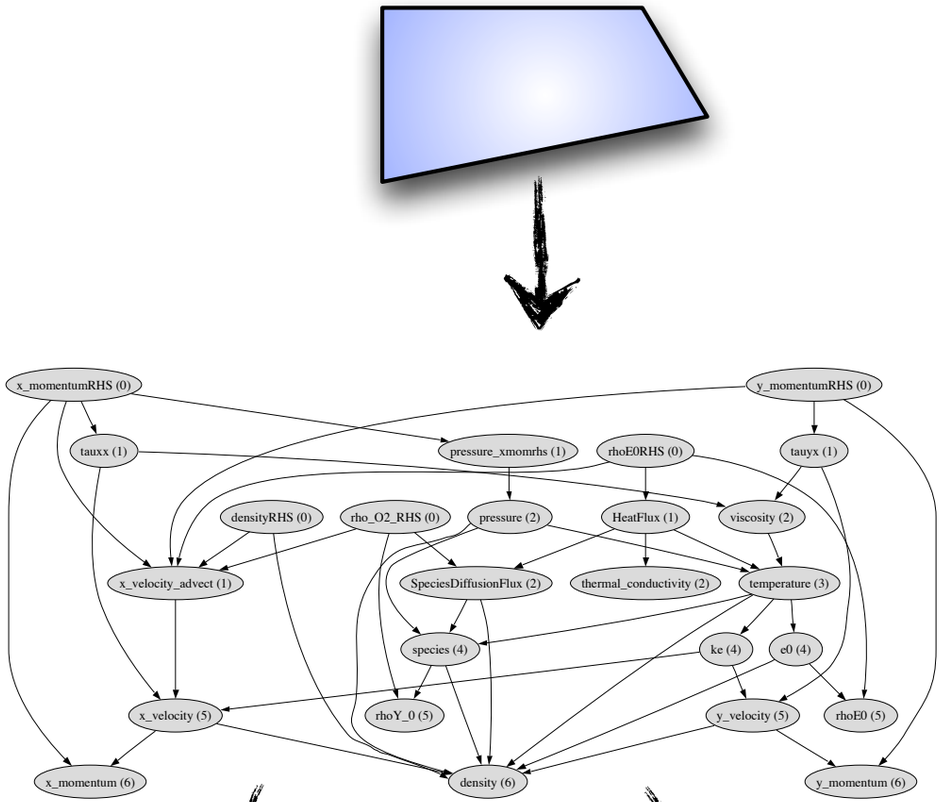
Hierarchical Parallelization

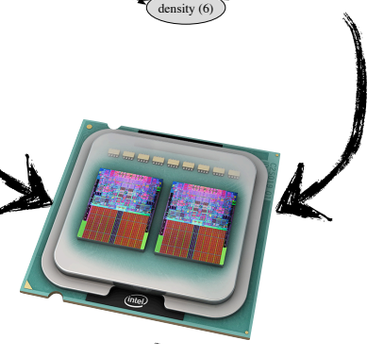
- Domain decomposition
  - data parallel (MPI)
- Algorithm decomposition
  - task parallel (threads)



Hierarchical Parallelization

- Domain decomposition
  - data parallel (MPI)
- Algorithm decomposition
  - task parallel (threads)
- Fine-grained field operations
  - data parallel (threads)



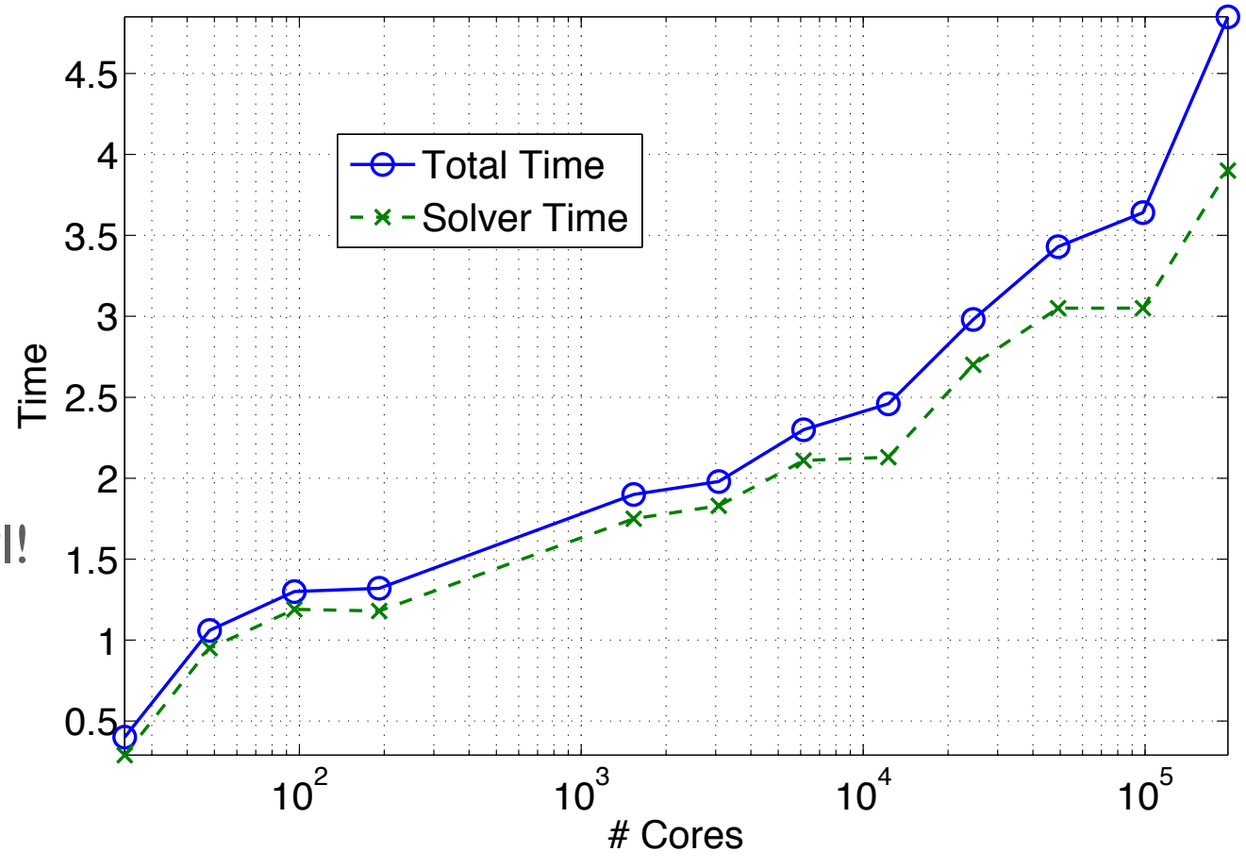


$$\nabla \cdot (\Gamma \nabla \phi) + s_\phi$$

data parallel per patch/workset

Current Scaling - Straight MPI ♻

- Efficiency:
  - MPI can scale to 200K cores (Jaguar)
    - Hypre PFMG solver, ~10 iterations required per timestep
  - Linear solver is dictating scalability
    - most of computation time is spent in linear solver
    - as we add more physics, more time will be spent outside the linear solver
- Implications:
  - Linear solvers must go multicore/GPU within MPI!
  - Consider algorithmic changes to eliminate dependency on linear solver?
- Multicore/accelerator implementations are a multiplier on MPI scalability.



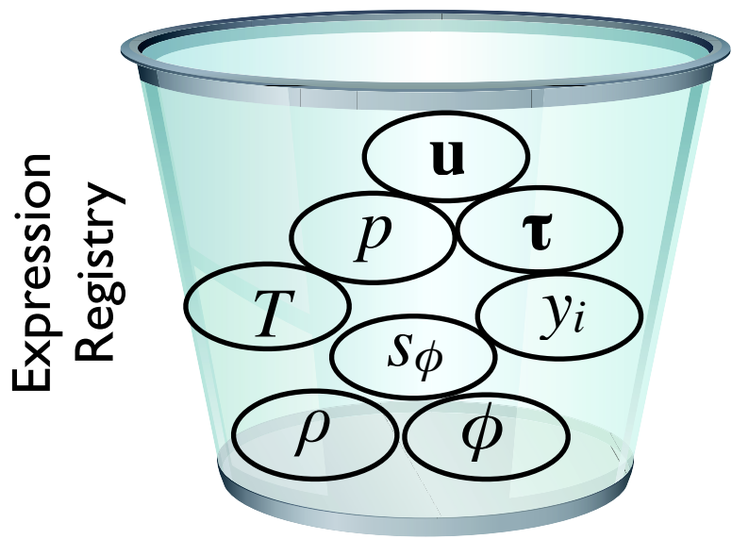
♻ Collaborative effort with Martin Berzins, funded by NSF awards OCI 0721659, PetaApps 0905068.

Task-Based Algorithm Decomposition

A Simple Example

- Register all expressions.
  - Each "expression" calculates one or more field quantities, and this is indicated to the registry.
  - Each expression advertises its *direct* dependencies

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot (\phi \mathbf{u}) + \nabla \cdot (\Gamma \nabla \phi) + s_\phi$$



Task-Based Algorithm Decomposition

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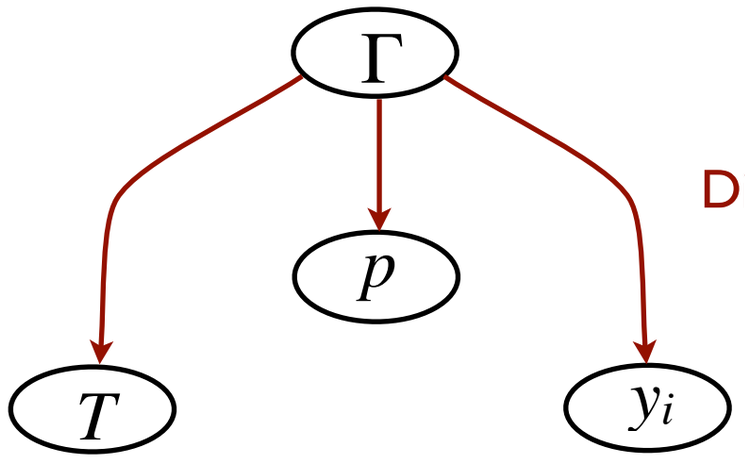
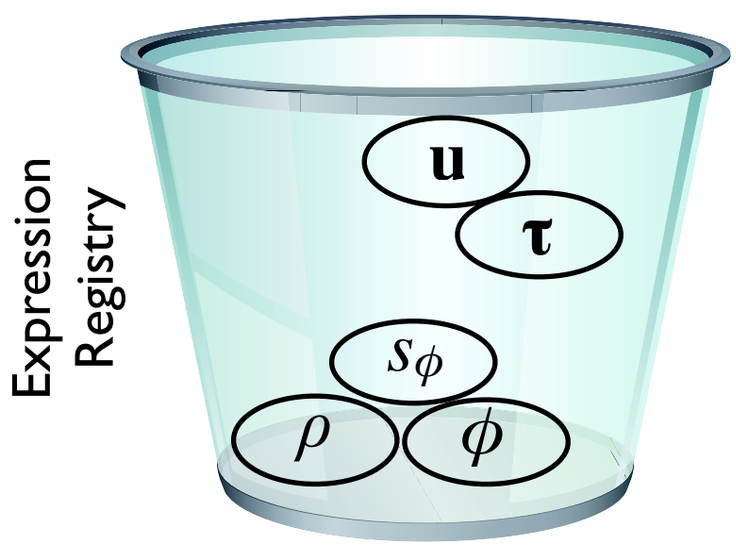
  - Each expression advertises its *direct* dependencies
- Determine a "root" expression & construct a graph.
  - All dependencies are discovered/resolved automatically and an algorithm is deduced.
- Highly localized influence of changes in models. Programmer need not know the "whole code" to make a local change.
- Not all expressions in the registry may be relevant/ used.

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot (\phi \mathbf{u}) + \nabla \cdot (\Gamma \nabla \phi) + s_\phi$$

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



Direct (expressed) dependencies.



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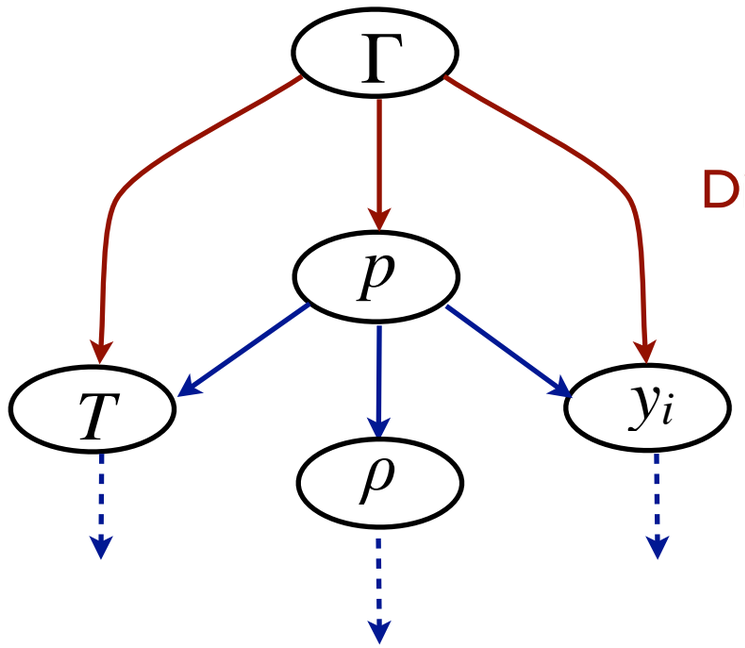
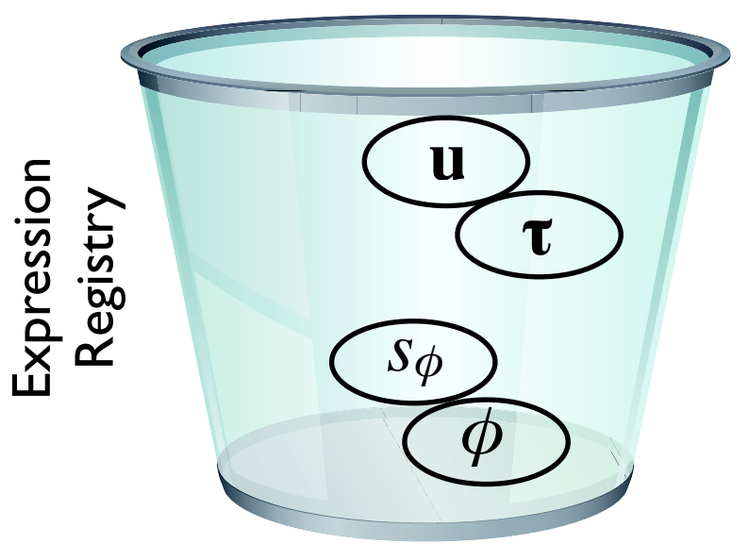


Direct (expressed) dependencies.

Indirect (discovered) dependencies.



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  - Highly localized influence of changes in models. Programmer need not know the "whole code" to make a local change.
  - Not all expressions in the registry may be relevant/ used.
- From the graph,
  - deduce storage requirements & allocate memory (externally to each expression).
  - iterate graph and bind memory.
  - schedule evaluation, ensuring proper ordering.

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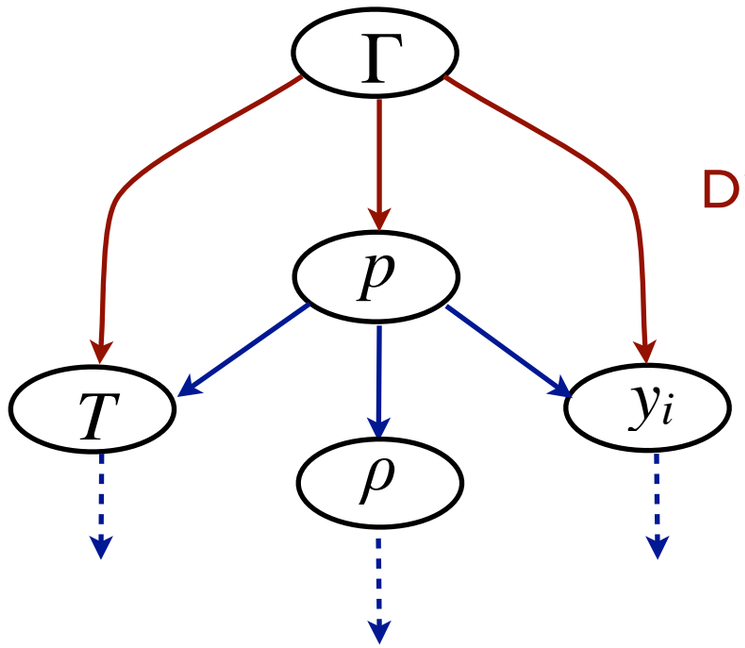

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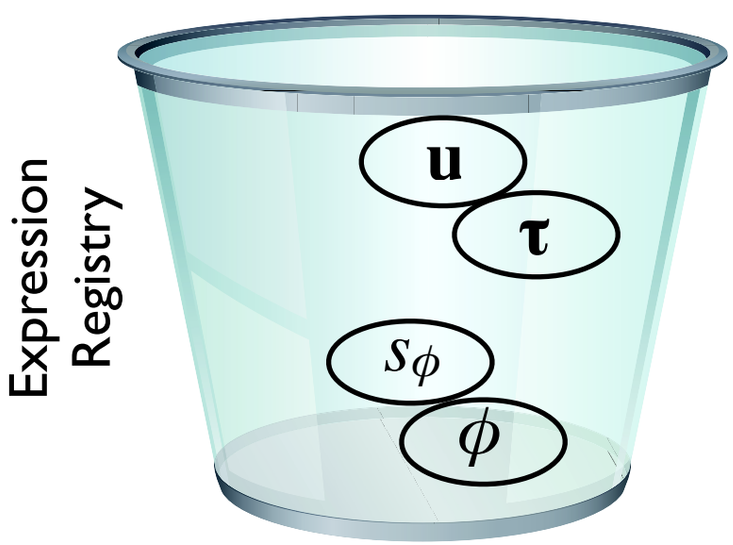

Additional Model Complexity

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{u})$$
$$\frac{\partial \rho \vec{u}}{\partial t} = -\nabla \cdot (\rho \vec{u}\vec{u}) - \nabla \cdot \tau - \nabla p + \rho \vec{g}$$
$$\frac{\partial \rho e_0}{\partial t} = -\nabla \cdot (\rho e_0 \vec{u}) - \nabla \cdot (p\vec{u}) - \nabla \cdot (\tau \vec{v}) - \nabla \cdot q$$
$$\frac{\partial \rho y_i}{\partial t} = -\nabla \cdot (\rho y_i \vec{u}) - \nabla \cdot \vec{J}_i + s_i$$

Additional Model Complexity

- Example: multiphase flows
  - Do we need logic in formulating each transport equation to indicate if "multiphase" is turned on?

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{u}) + s_\rho$$
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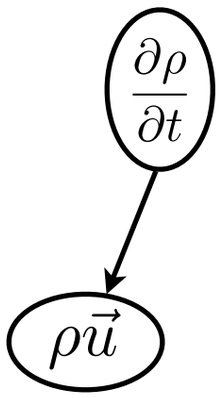

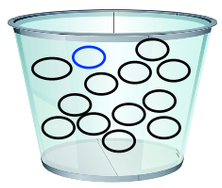

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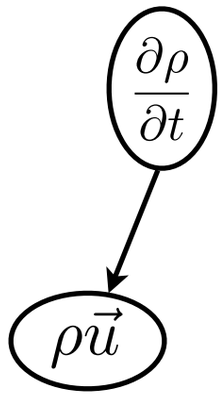
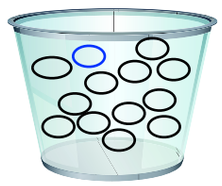
- "Attach" a dependency to an expression.
  - Allows "push" coupling rather than "pull" coupling
  - Physics that knows about coupling (particle transport) injects appropriate coupling terms into gas-phase solver.
  - Full dependency structure is maintained; no "code creep" from additional models.





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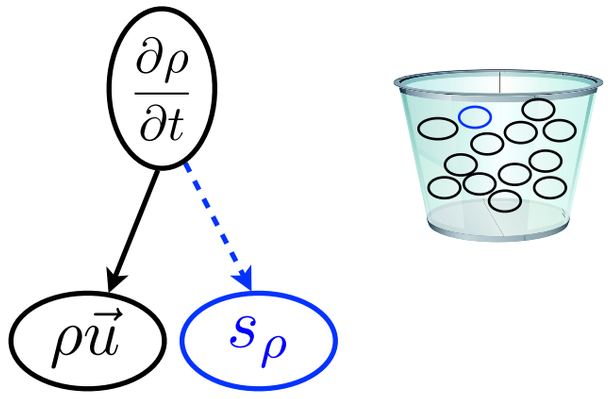


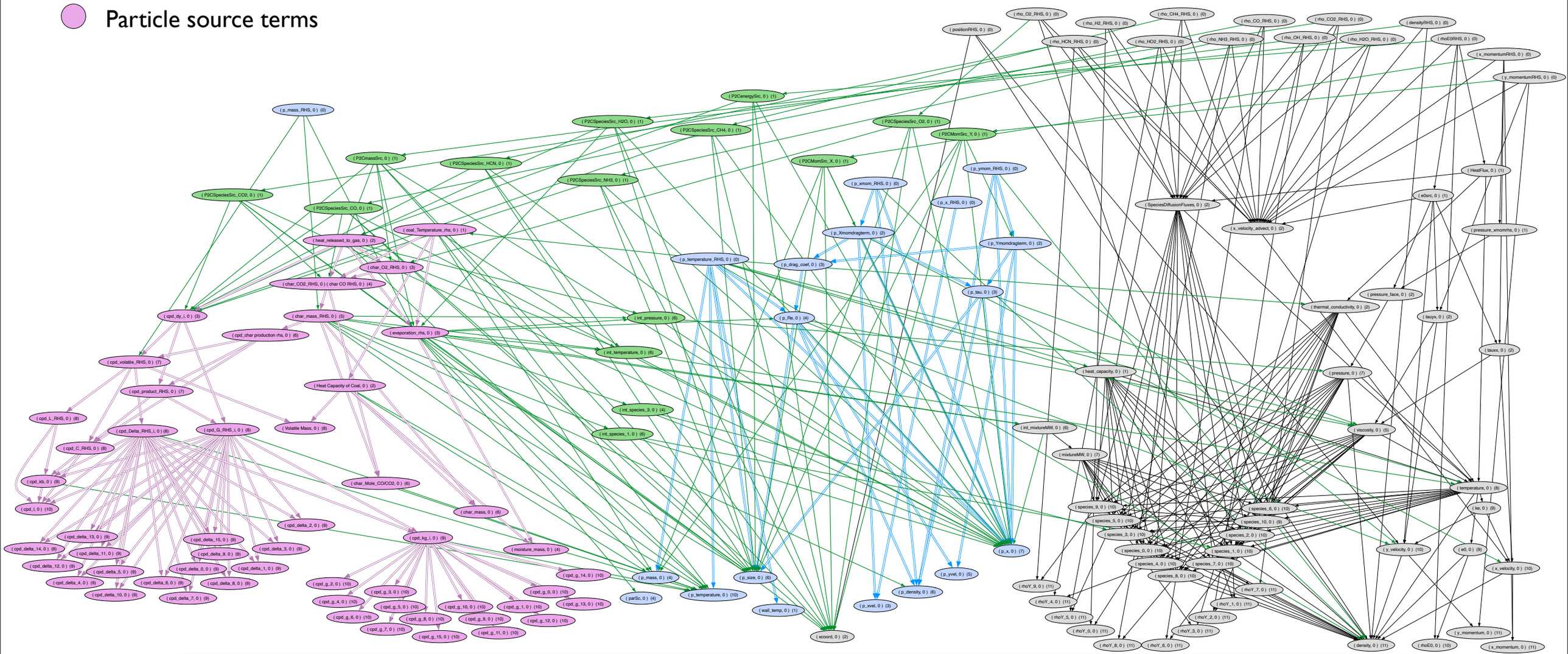

```
registry->attach_dependency( rhoRHS, srho, ADD );
```

$\partial \varrho / \partial t$ doesn't directly advertise a dependency on s_ϱ.

Example Graph - Coal Combustion/Gasification

- Gas phase terms (CO/H2 combustion - moving to methane...)
- Particle evolution terms
- Particle - gas coupling terms
- Particle source terms

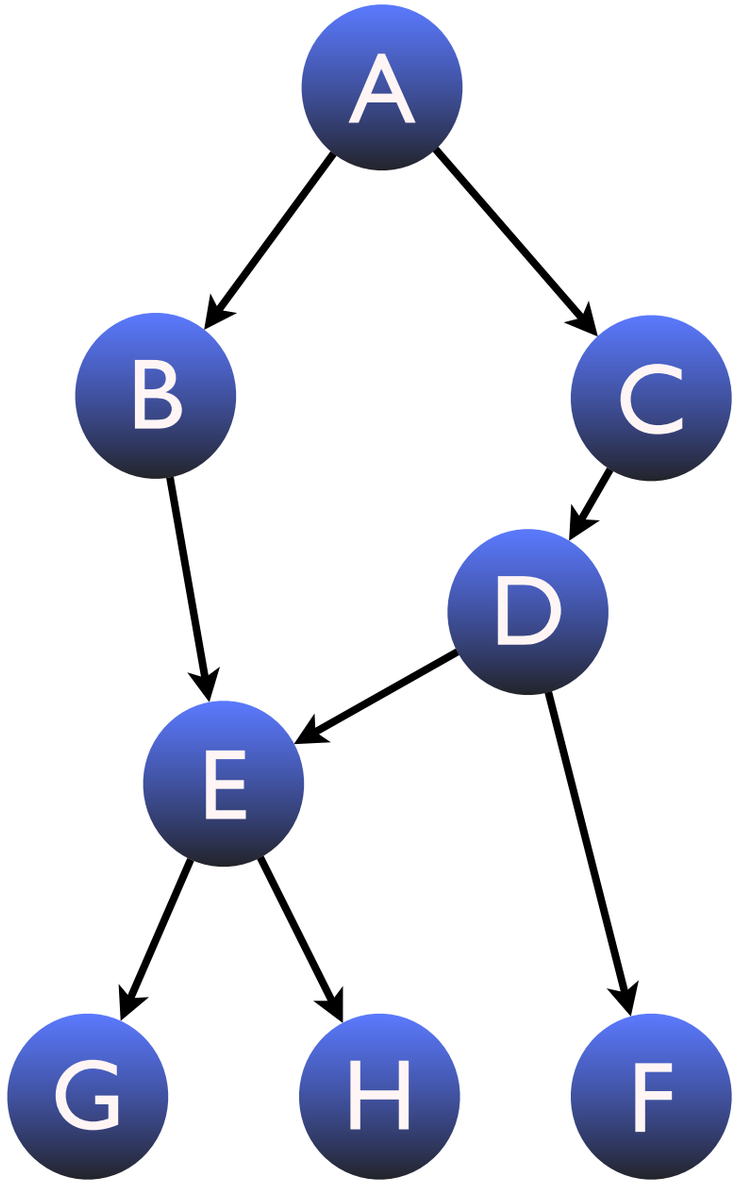
15 Gas-phase PDEs,
~25 ODEs per particle.



NO modification to gas-phase code to get 2-way coupling on mass, momentum, energy!

Multicore Scheduling

- "Bottom" nodes are placed in execution queue.
- When a node completes, its "wait count" is decremented.
- When all of a node's "children" are done (wait count=0) it is placed in the priority execution queue.
  - priority determined to optimize graph execution time.
  - backfilling naturally occurs (particularly for broad graphs) while "heavy" nodes execute.
  - resources may be dynamically migrated between thread pool associated with task graph to threads associated with data-parallel execution (within a node)



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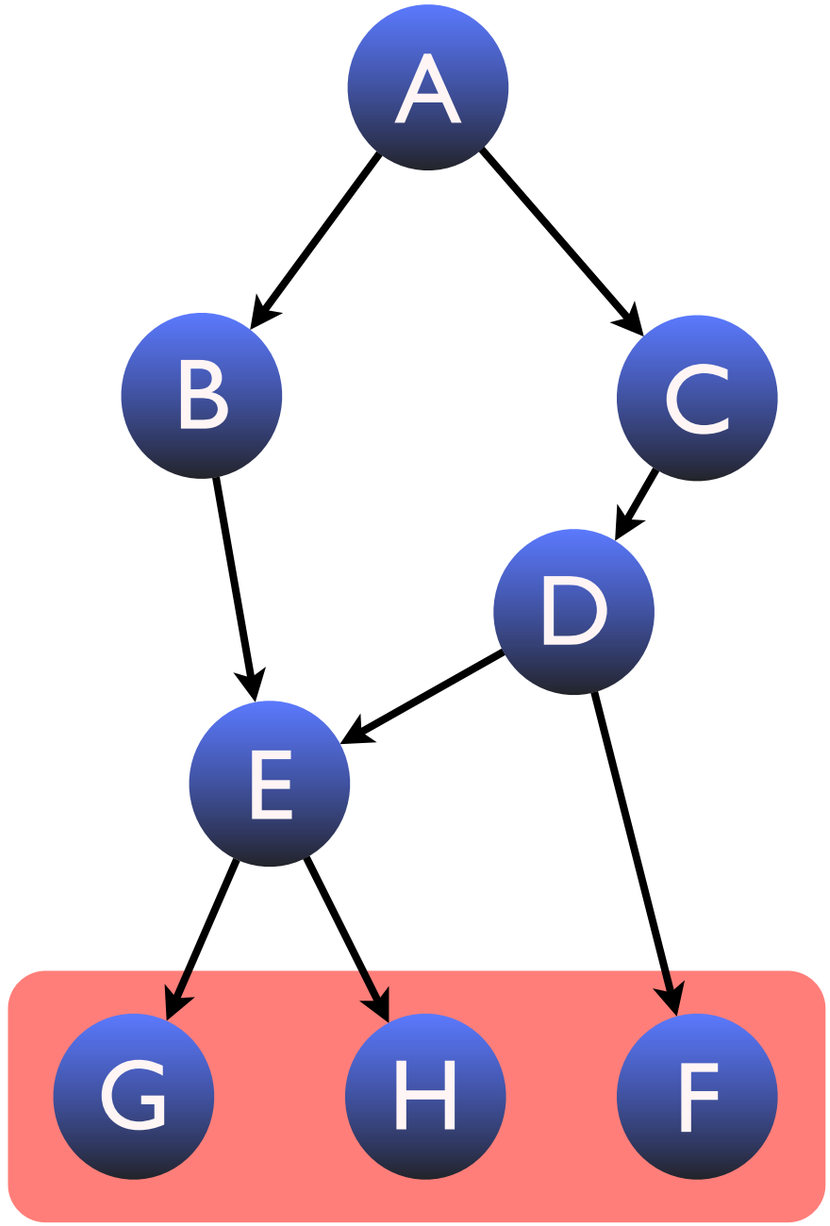

Prioritize G, H because they are "deeper" than F.

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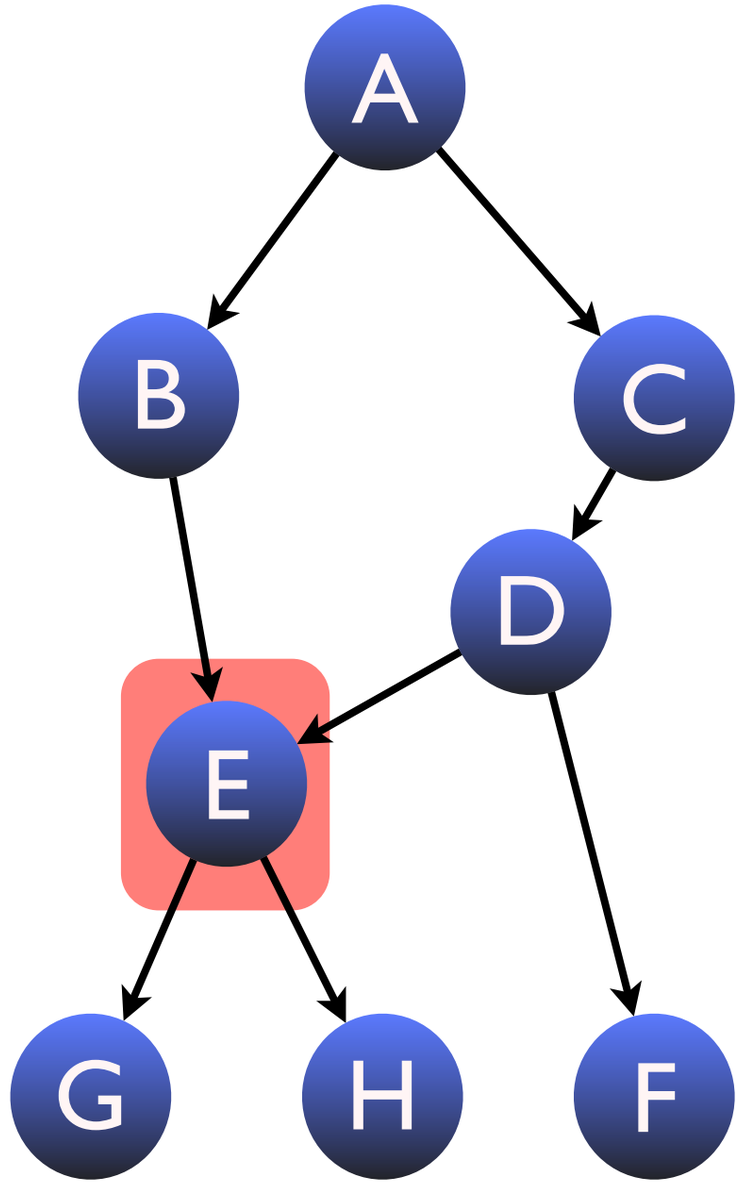

Serialization point - push resources into data parallel on E.

Multicore Scheduling

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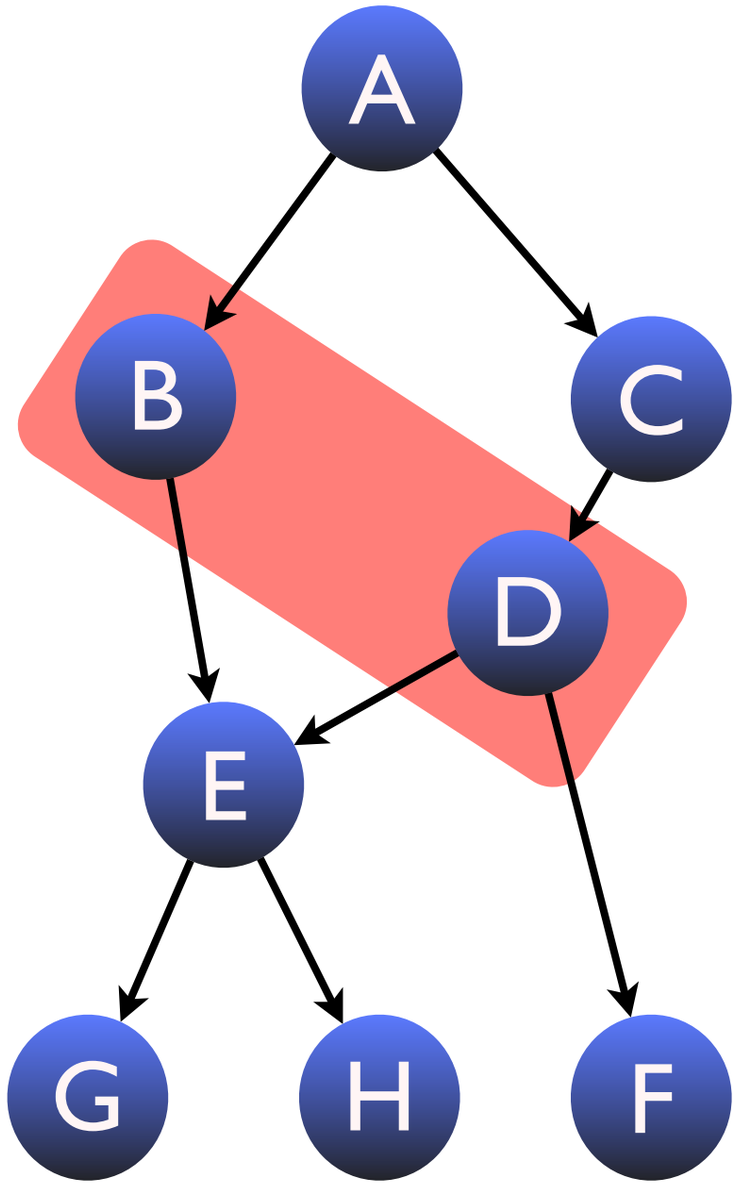

Prioritize D (may push resources into "D" if possible)

Multicore Scheduling

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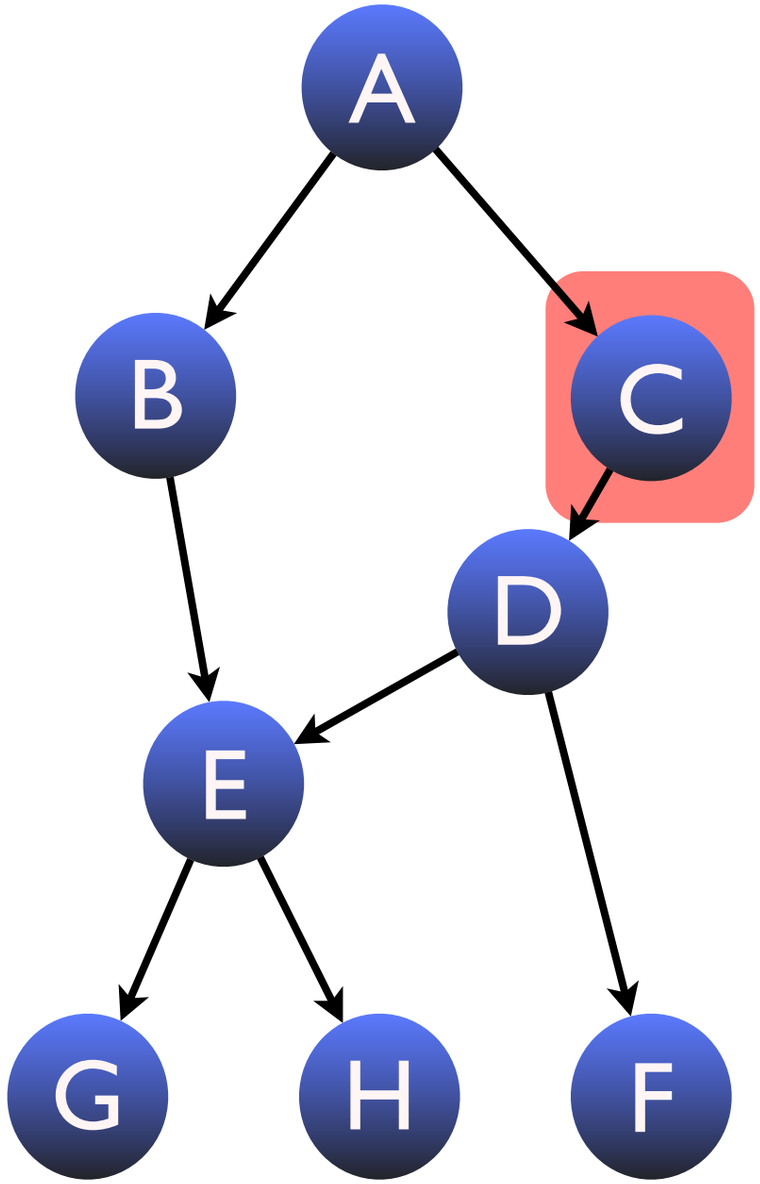

Serialization point - push resources into data parallel on C.

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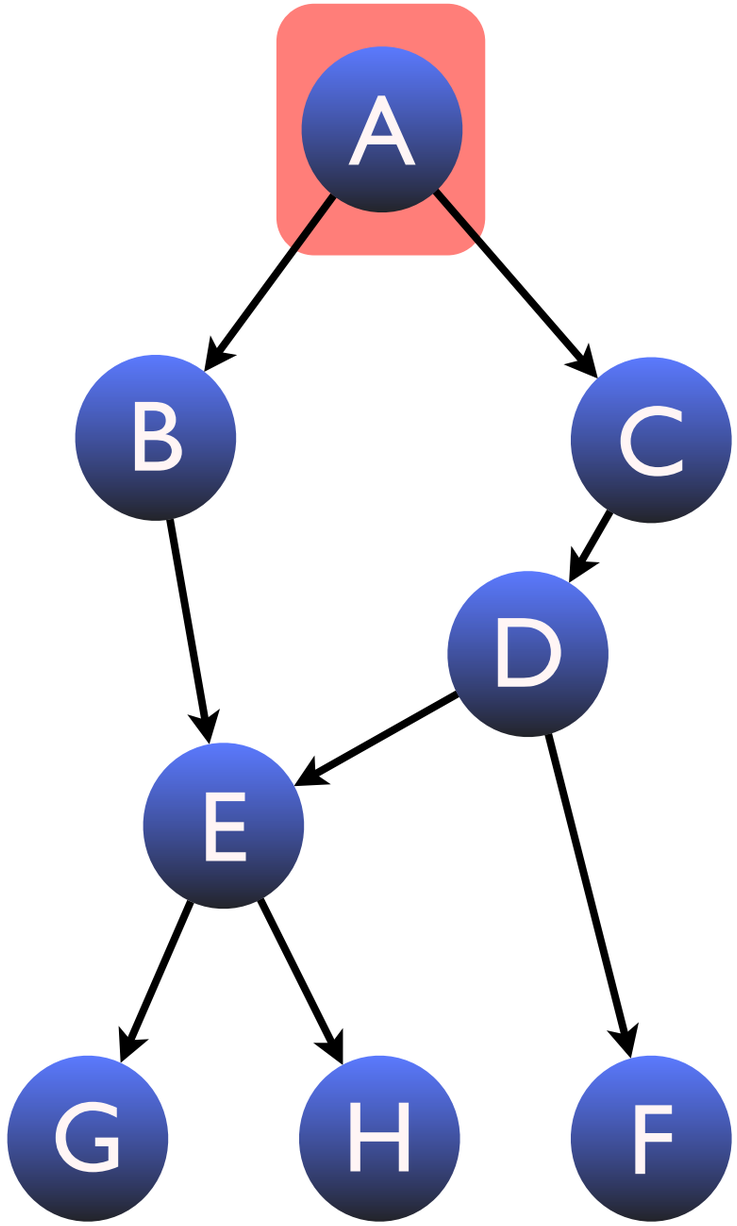
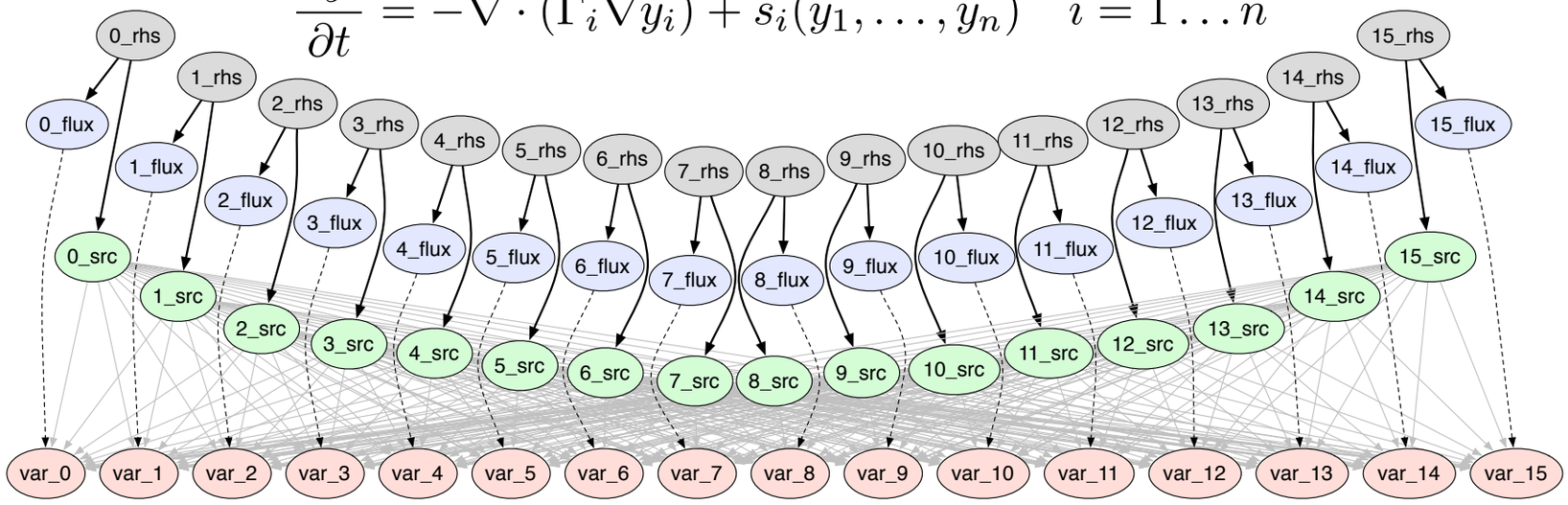


Serialization point - push resources into data parallel on A.

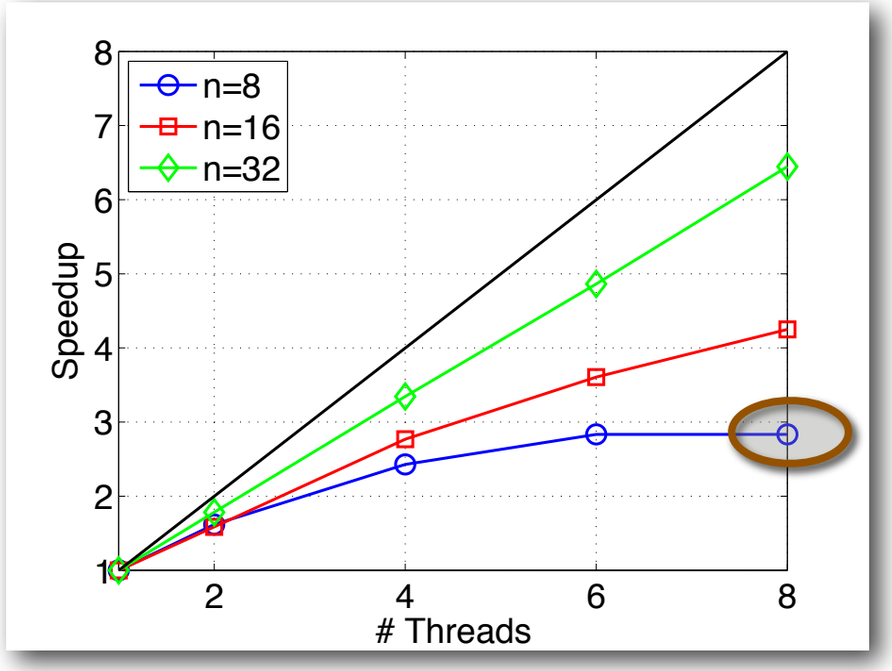
Idealized Scaling Example (Task Parallel)

$$\frac{\partial y_i}{\partial t} = -\nabla \cdot (\Gamma_i \nabla y_i) + s_i(y_1, \ldots, y_n) \quad i = 1 \ldots n$$



Graph analysis indicates theoretical parallelizability and speedup.

n	$\mathcal{P}$	$\mathcal{S}_\infty$
8	0.89	7.5
16	0.94	13.7
32	0.97	28.6



- Broad graphs required for task-based parallelism.
- Currently not obtaining close to theoretical scalability - cache issues?
- To obtain many-core scalability, we need to expose concurrency within each task!

P. K. Notz, R. P. Pawlowski, and J. C. Sutherland, "Graph-based software design for managing complexity and enabling concurrency in multiphysics PDE software," *ACM Transactions on Mathematical Software*, to appear, 2012

Granularity & Multicore Scaling (Data Parallel)

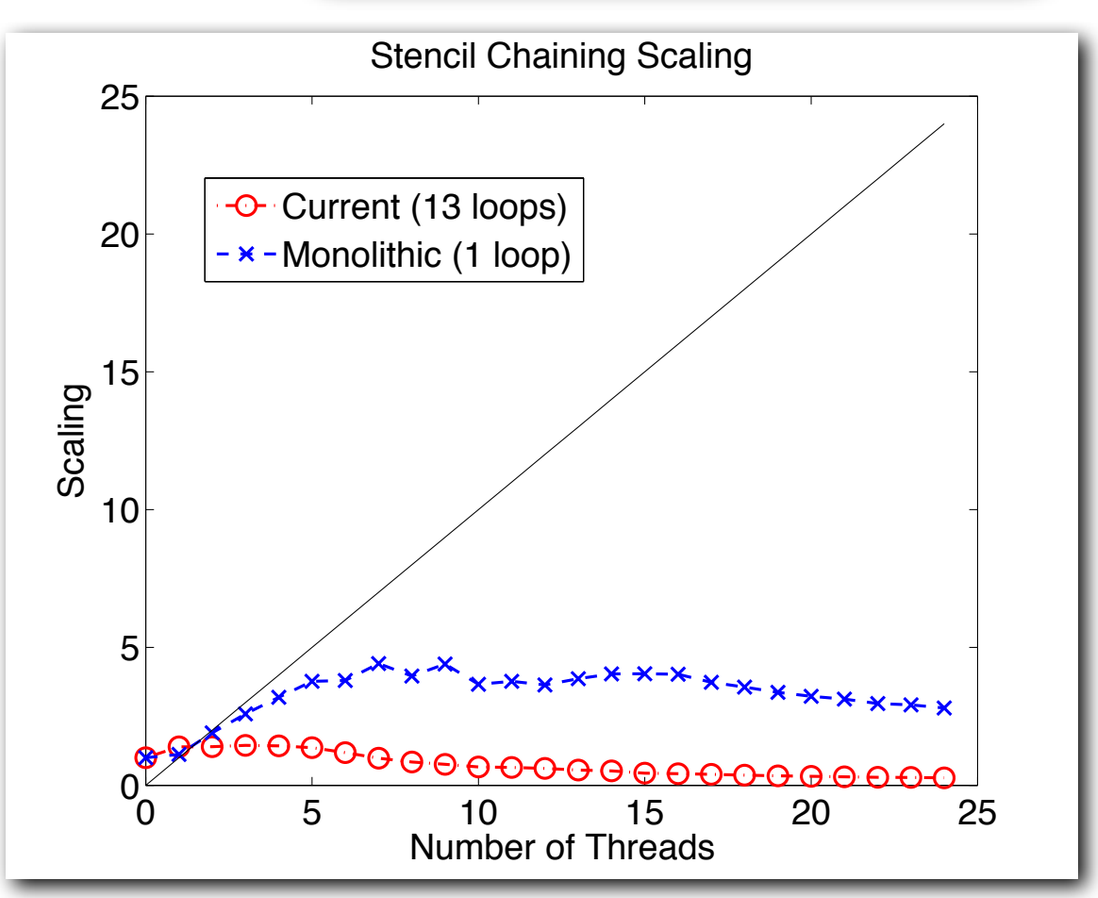
$$\frac{\partial \phi}{\partial t} = -\frac{\partial}{\partial x}\left(-\lambda \frac{\partial \phi}{\partial x}\right) - \frac{\partial}{\partial y}\left(-\lambda \frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(-\lambda \frac{\partial \phi}{\partial z}\right)$$

"Naive" implementation

1. Calculate λ
2. Interpolate λ to faces (3 loops)
3. Calculate gradient of ϕ at faces (3 loops)
4. Multiply $\partial\phi/\partial x_i$ by λ (3 loops)
5. Calculate divergence (3 loops)
6. Form full RHS (1 loop)

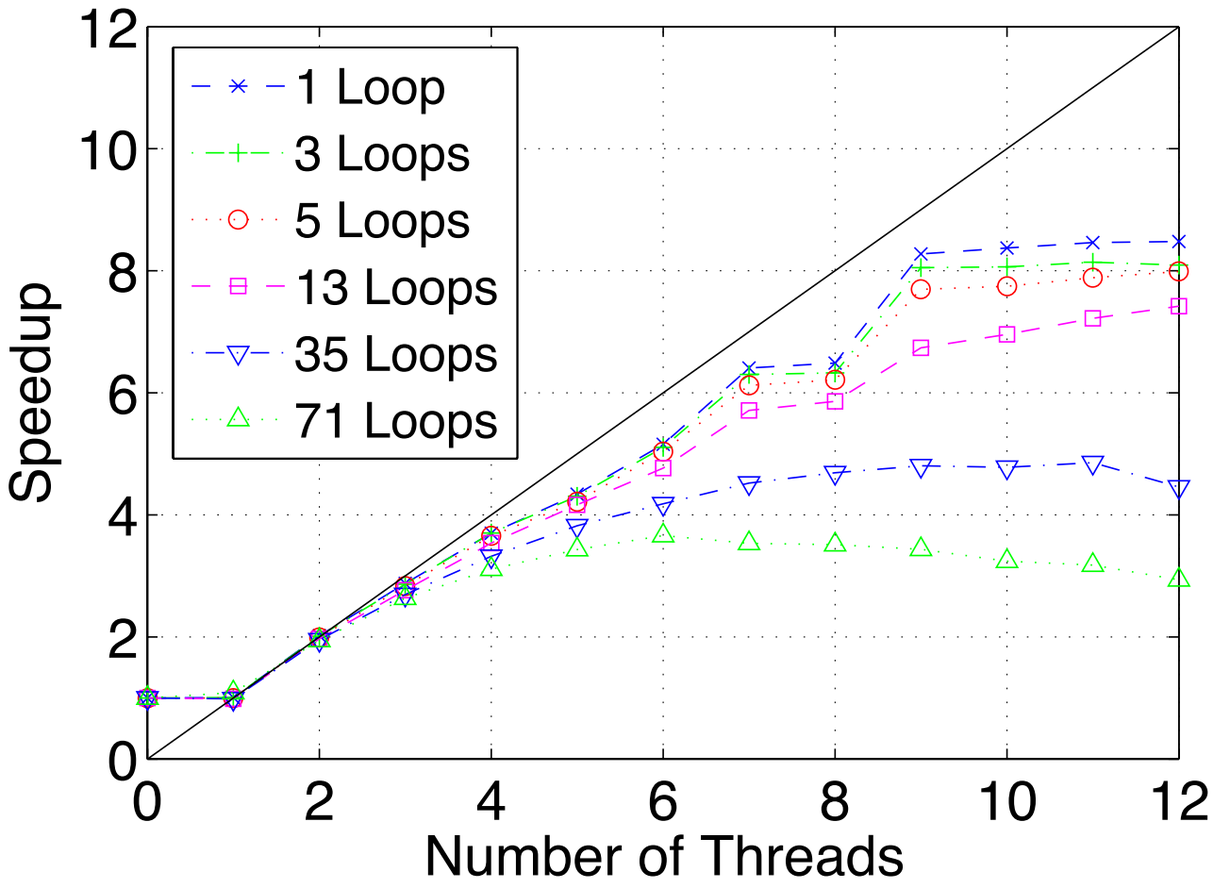
Loop Fusing

1 loop, λ and $\partial\phi/\partial x_i$ held as temporaries on inner loops.



- Cache contention is a real issue (work/write)
- Loop fusing is important (works against traditional abstraction)
- DSLs can help ease this pain significantly!

Domain-Specific Languages



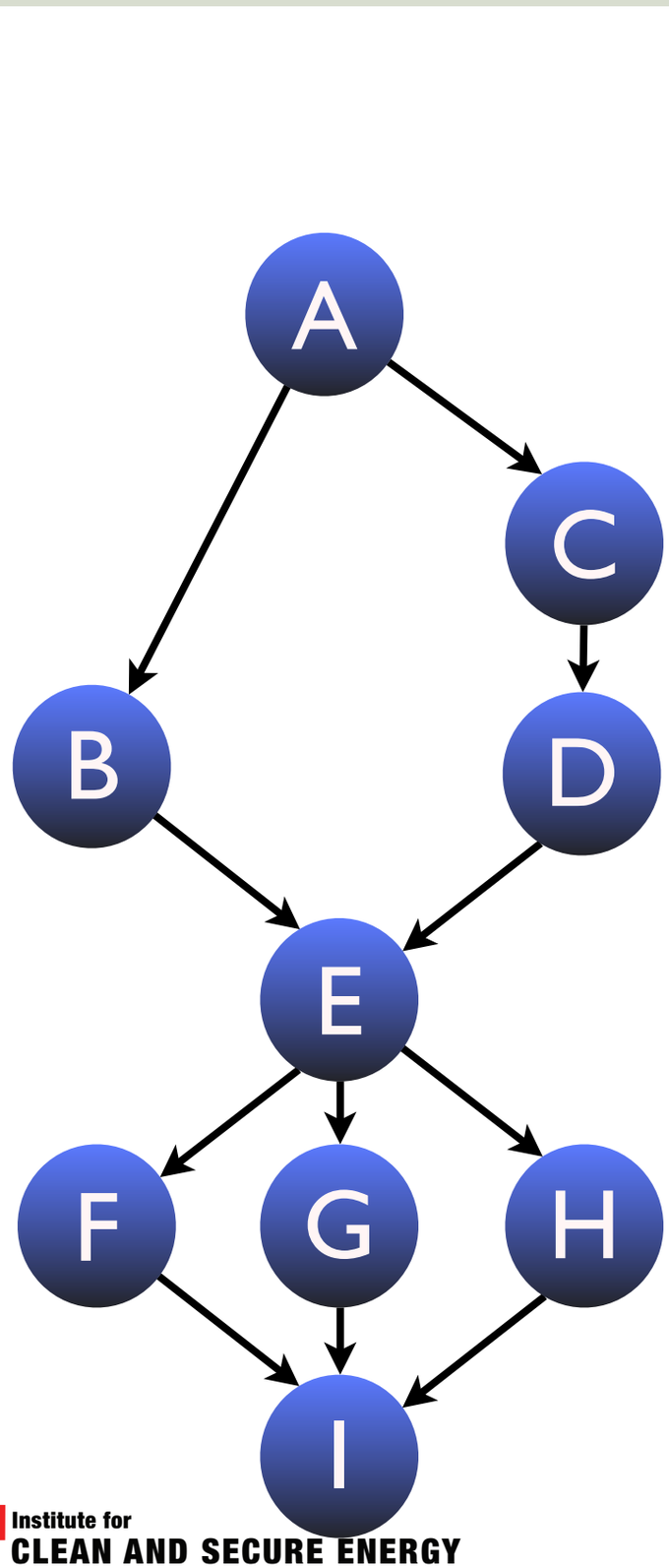
- Need "loop fusing" - more work per loop, fewer loops.
- Many threads overload memory bus.

$$\frac{\partial}{\partial x}\left(\Gamma\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\Gamma\frac{\partial\phi}{\partial z}\right)+s_\phi$$

```
rhs <<= Dx( Rx(Gamma) * Gx(phi) )
      + Dy( Ry(Gamma) * Gy(phi) )
      + Dz( Rz(Gamma) * Gz(phi) )
      + Sphi
```

DSL hides details of implementation - fast refactors

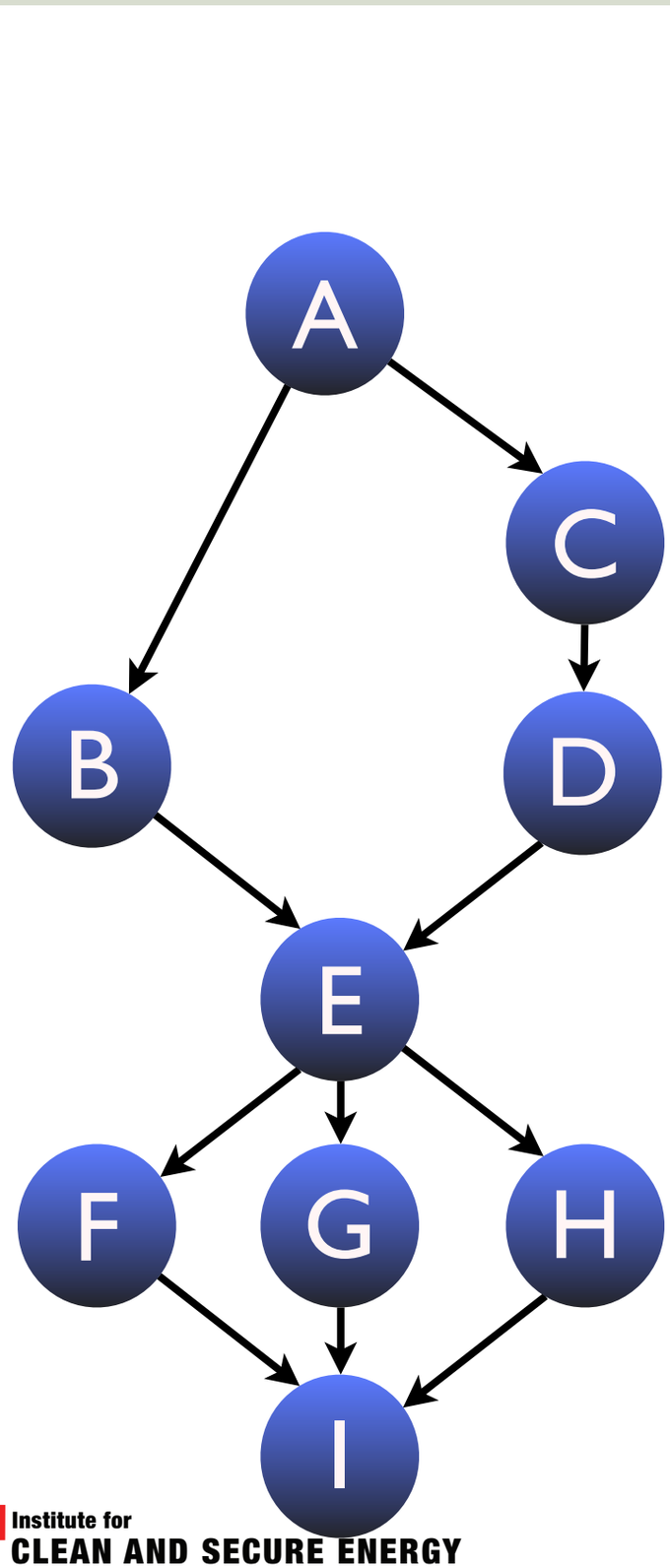
Memory Management - Pool Allocation



Static fields

Dynamic fields

Memory Management - Pool Allocation



Stage 1

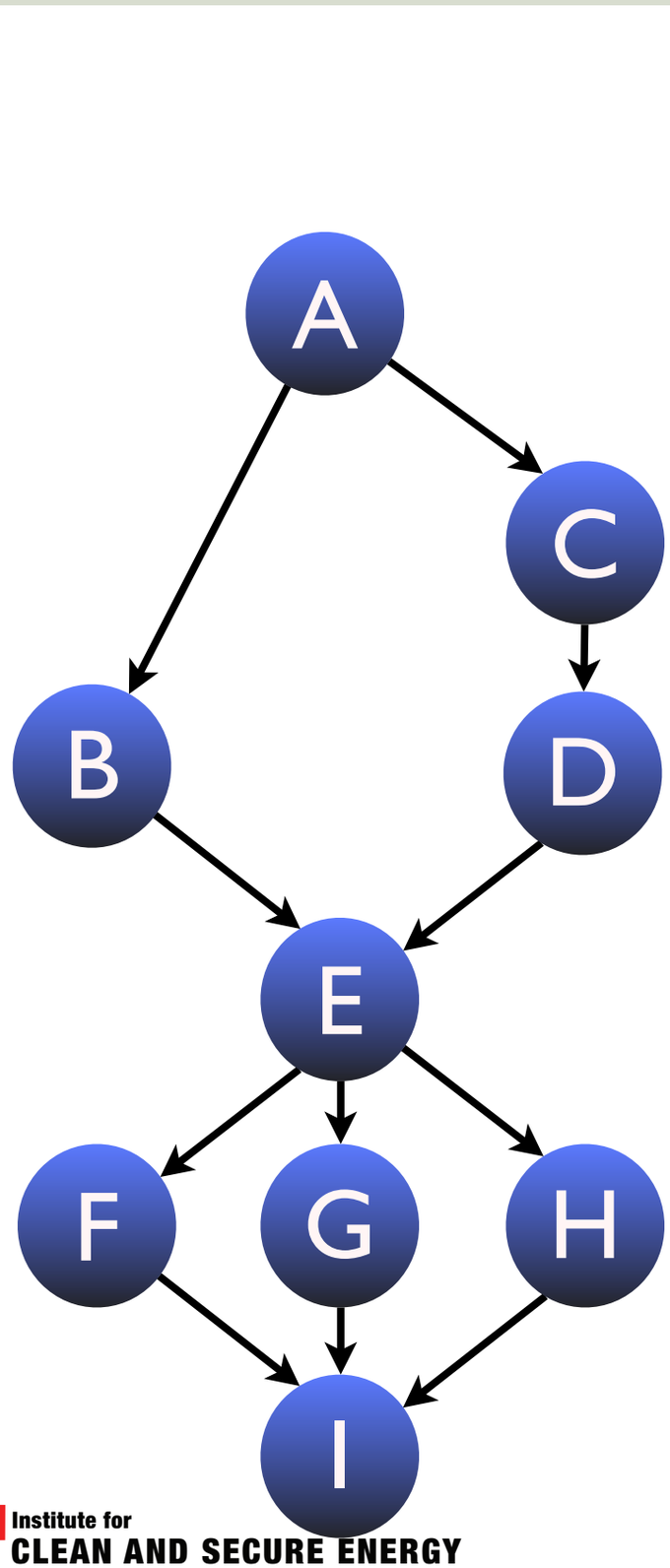
'I', 'A' allocated statically

Static fields

I A

Dynamic fields

Memory Management - Pool Allocation



Static fields

I A

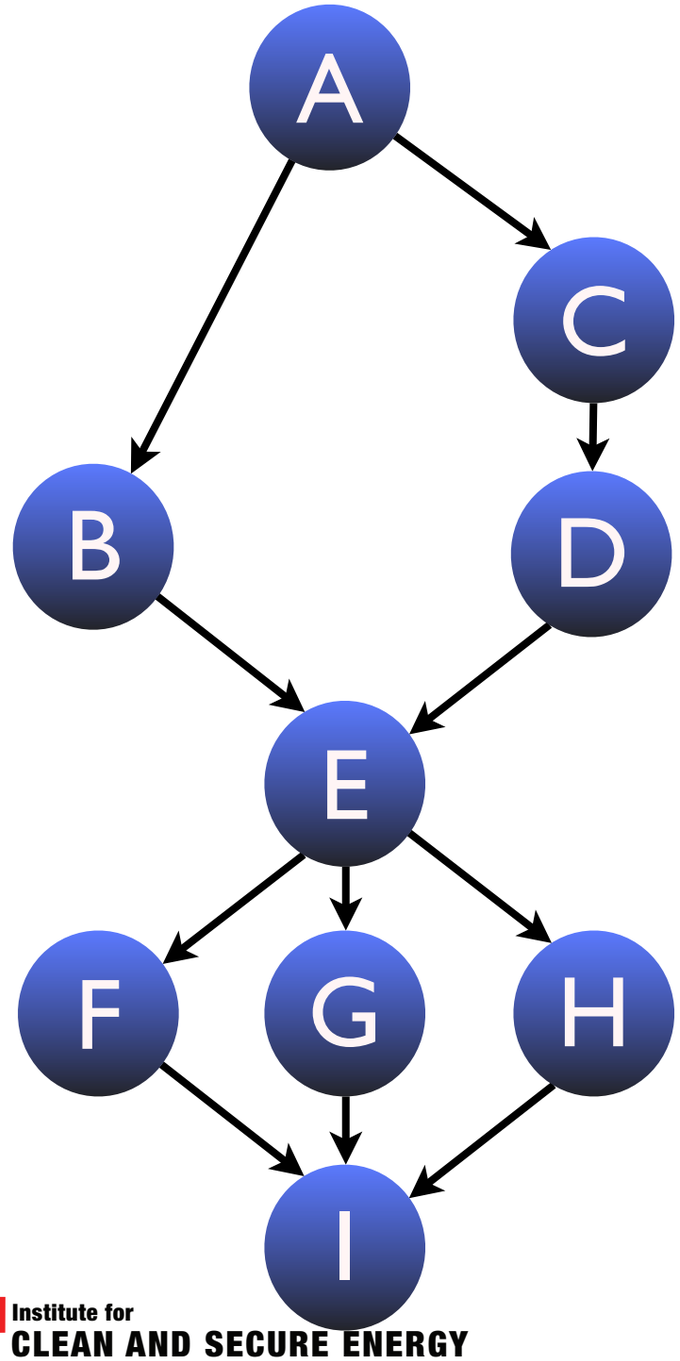
Dynamic fields

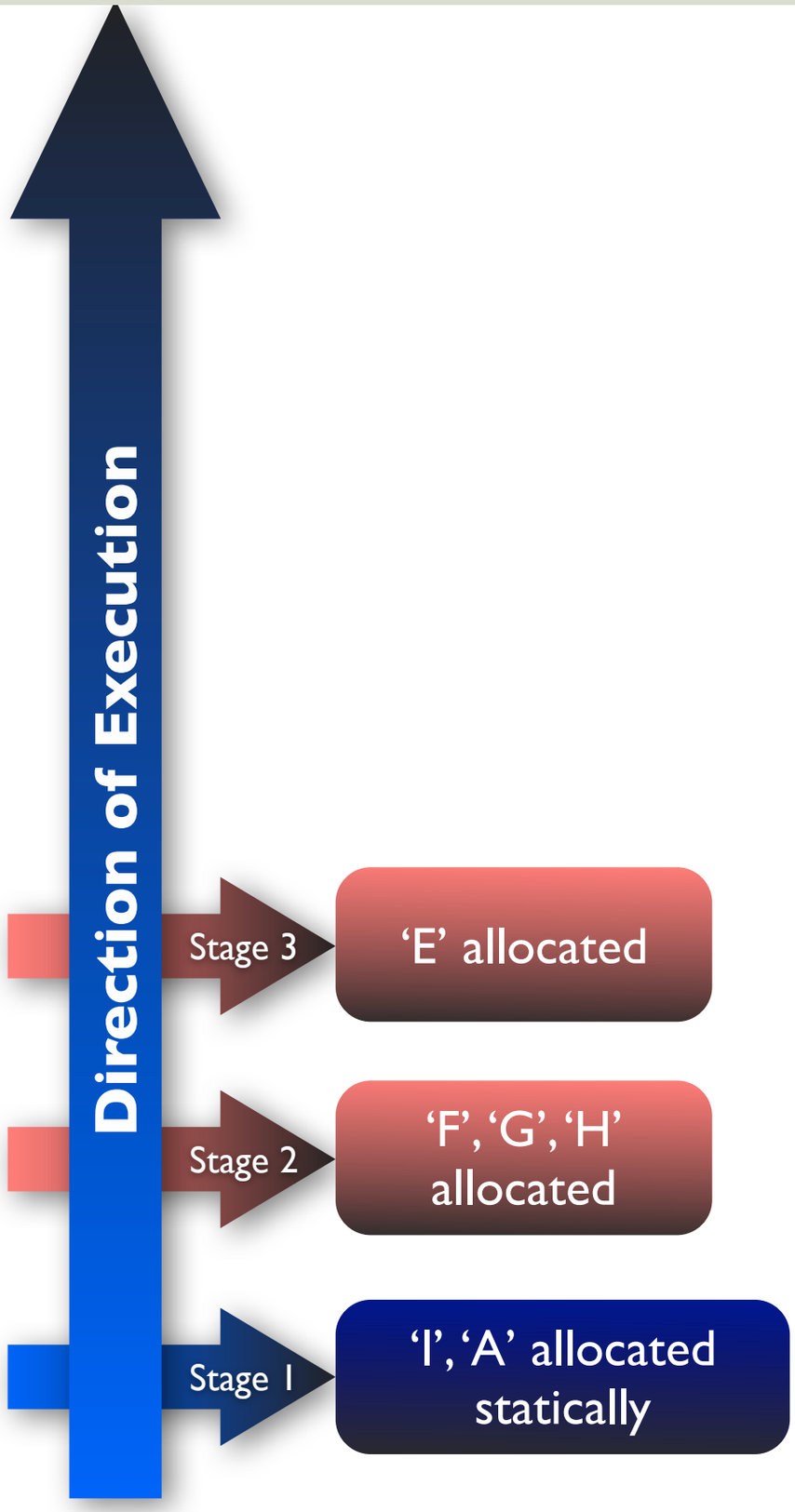
F G H

Stage 2 → 'F', 'G', 'H' allocated

Stage 1 → 'I', 'A' allocated statically

Memory Management - Pool Allocation





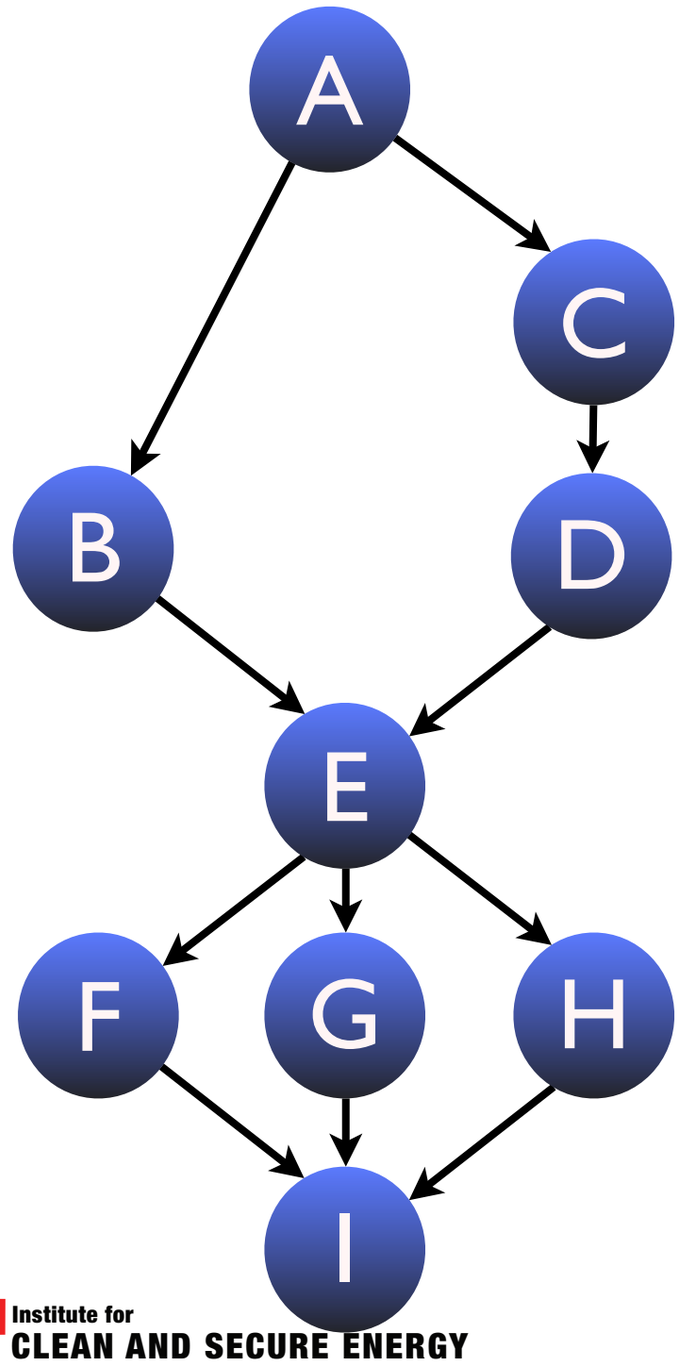
Static fields

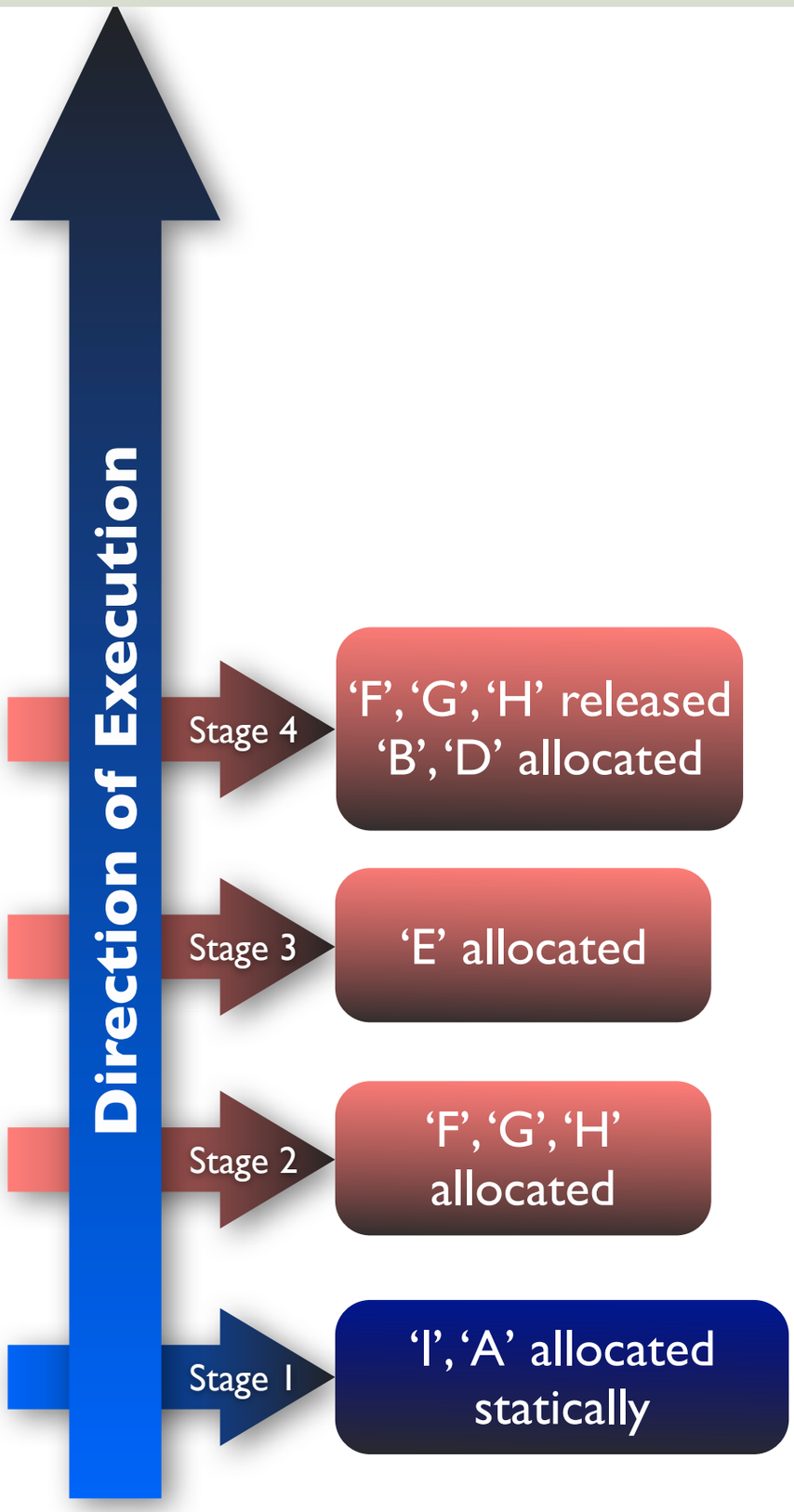
I A

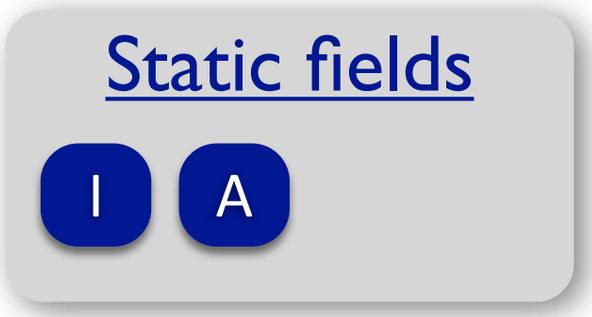
Dynamic fields

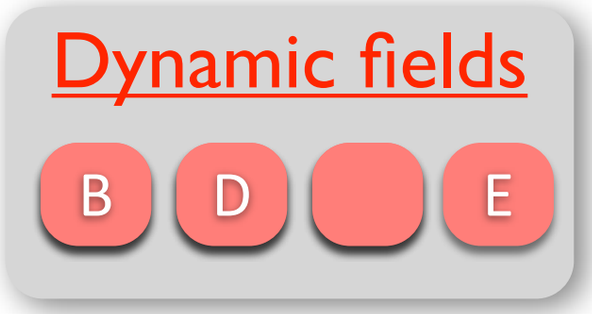
F G H E

Memory Management - Pool Allocation

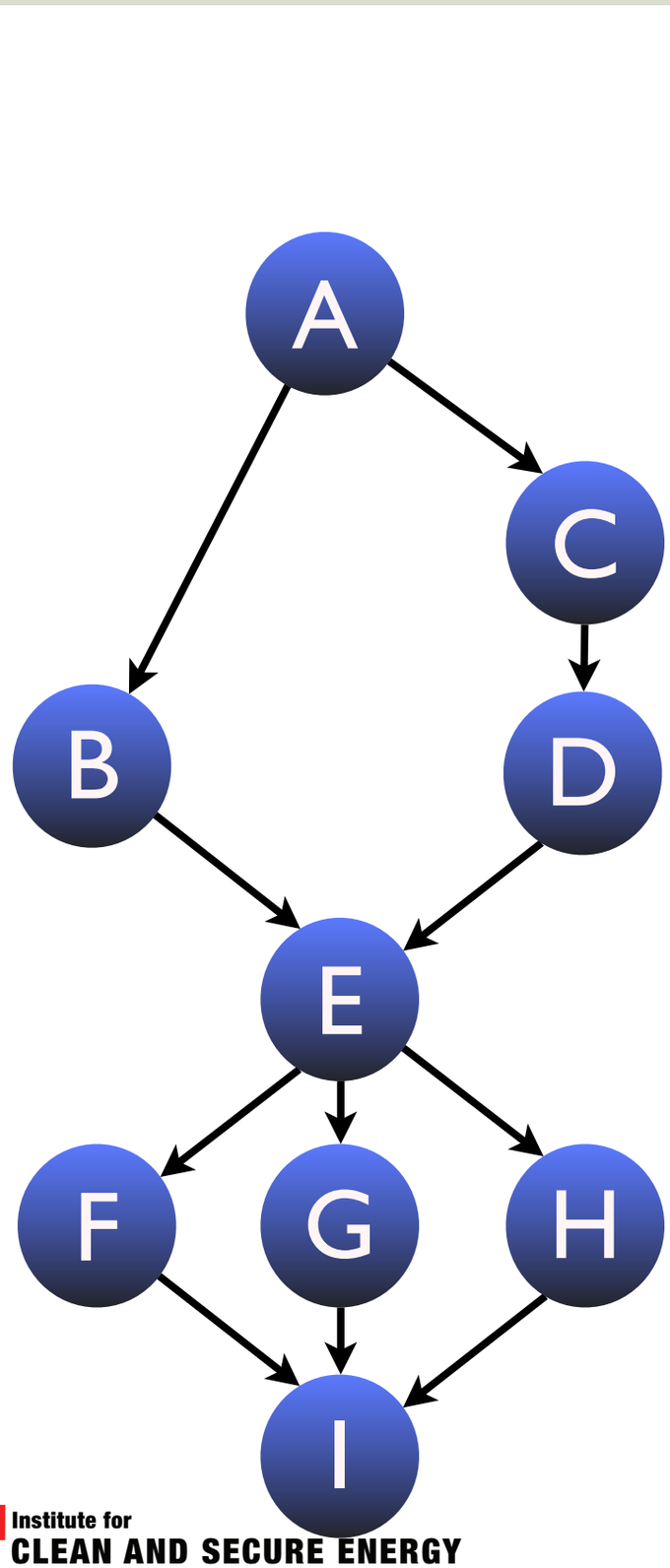


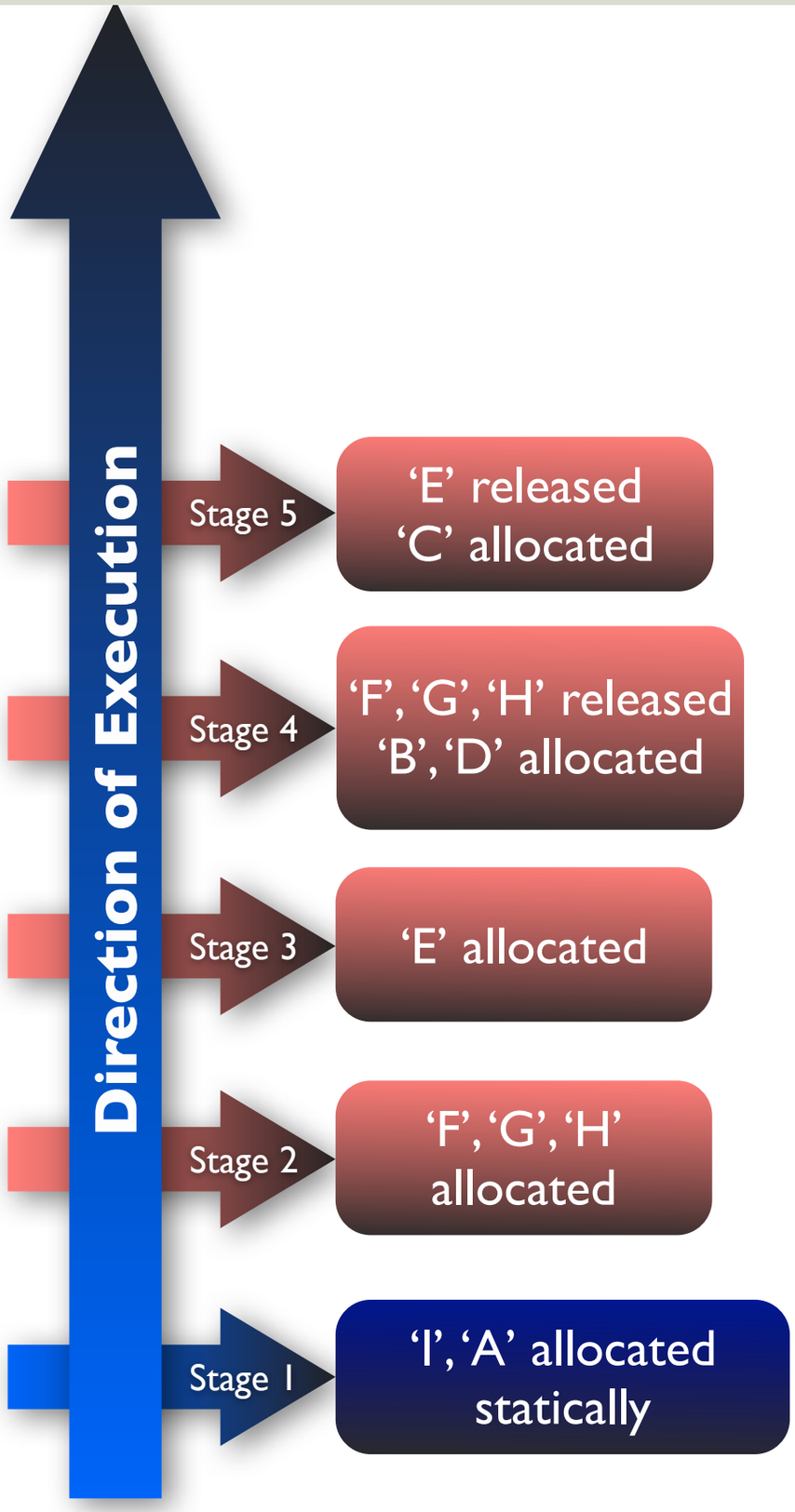


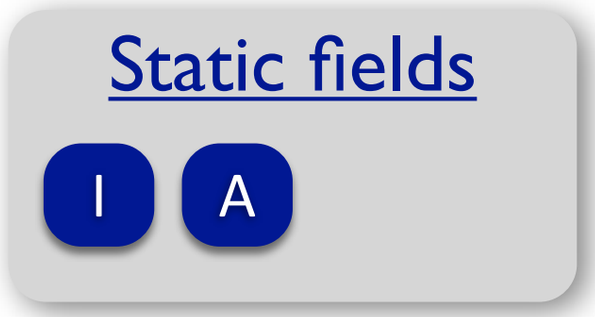


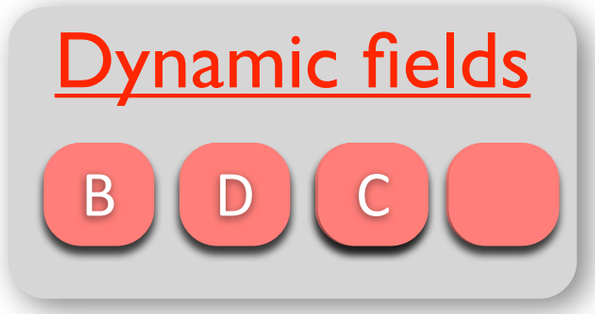


Memory Management - Pool Allocation

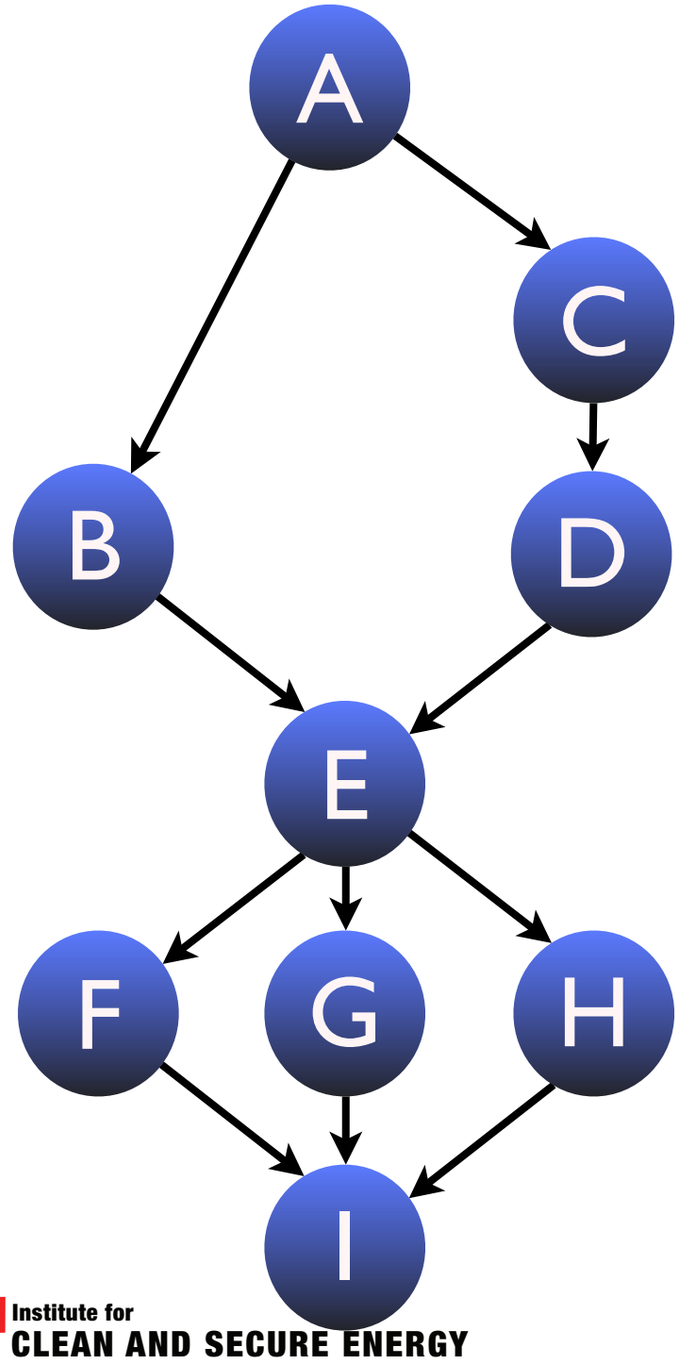


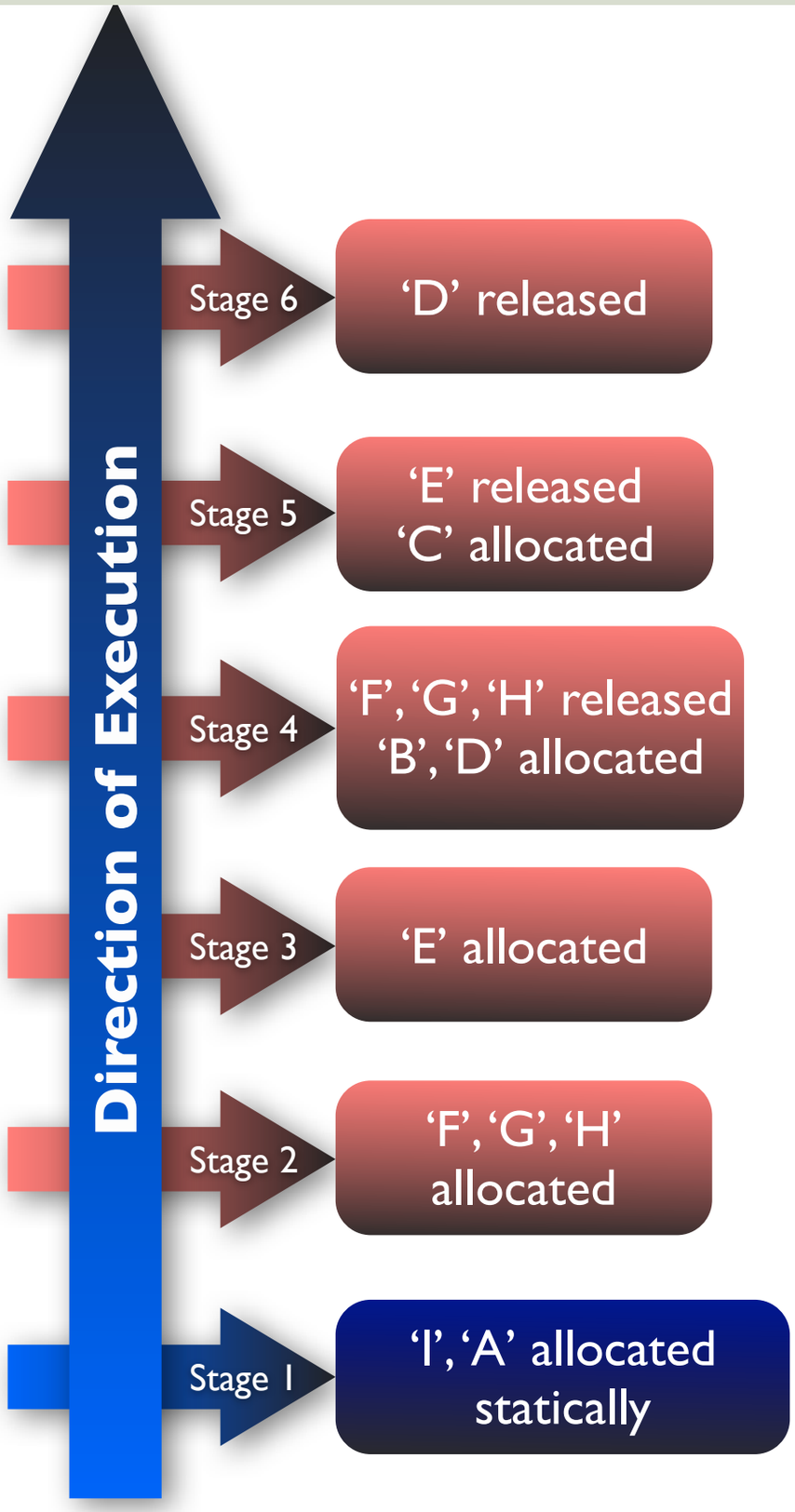


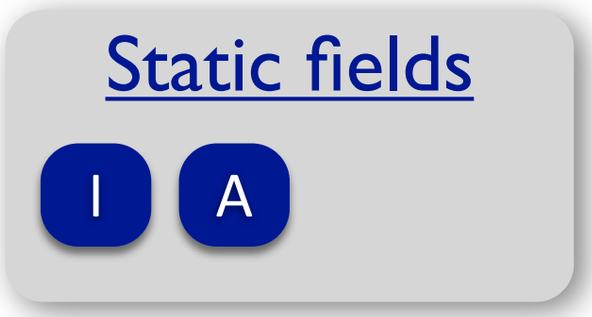


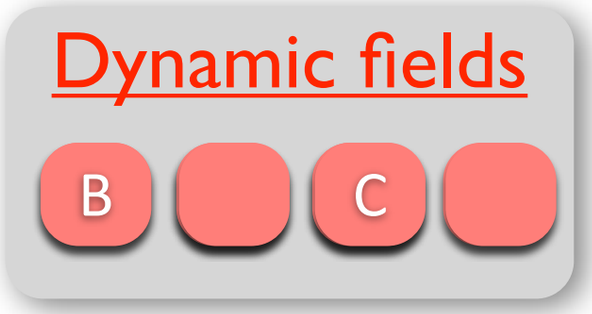


Memory Management - Pool Allocation



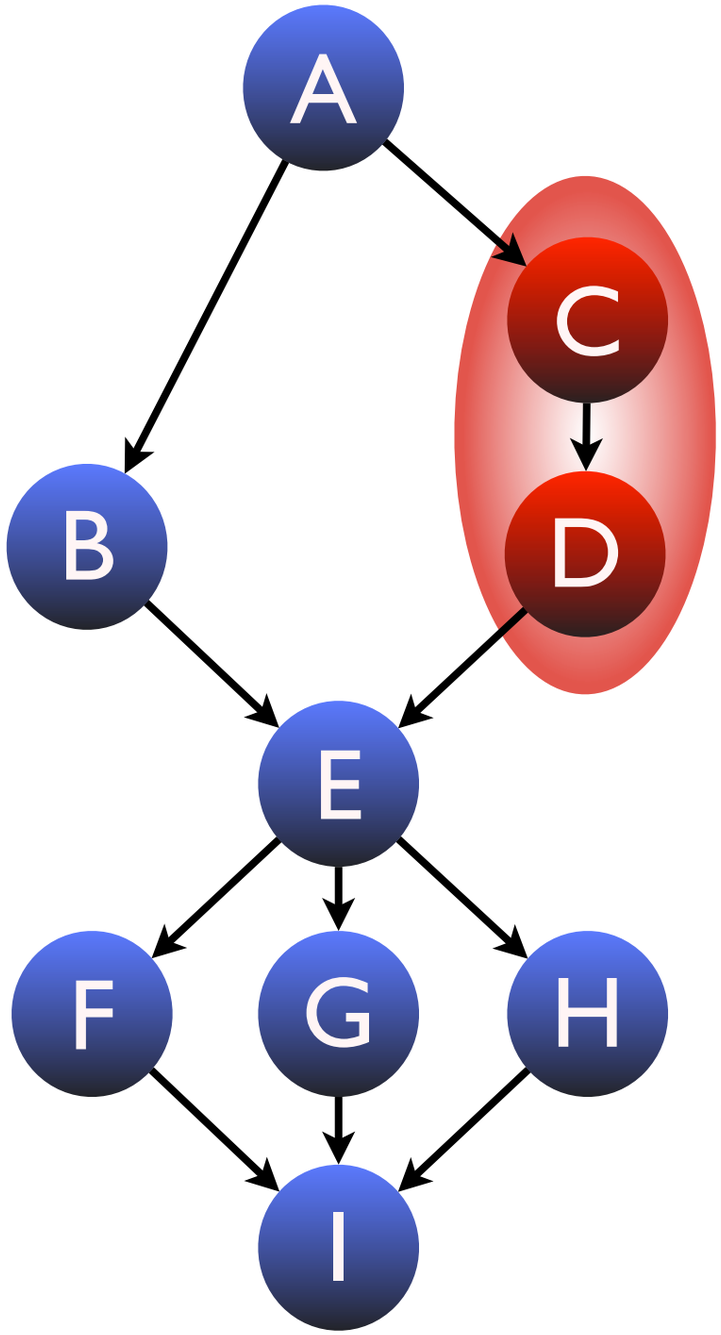






For deep graphs, this can result in very significant memory savings.

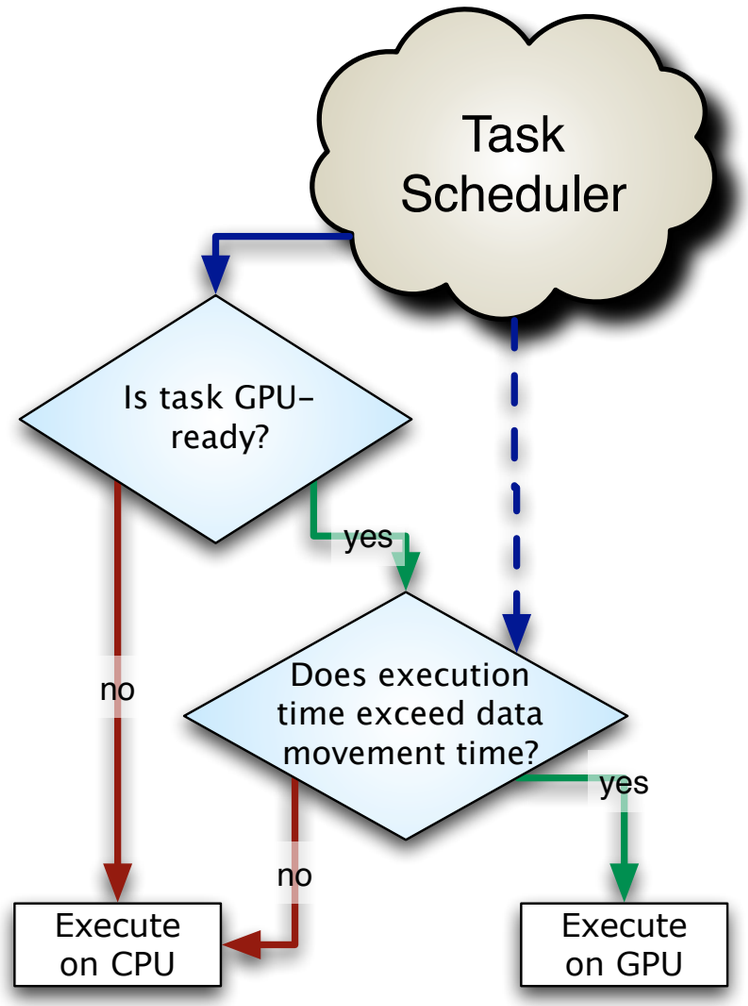
Current Work - Hybrid CPU/GPU



GPU - enabled nodes

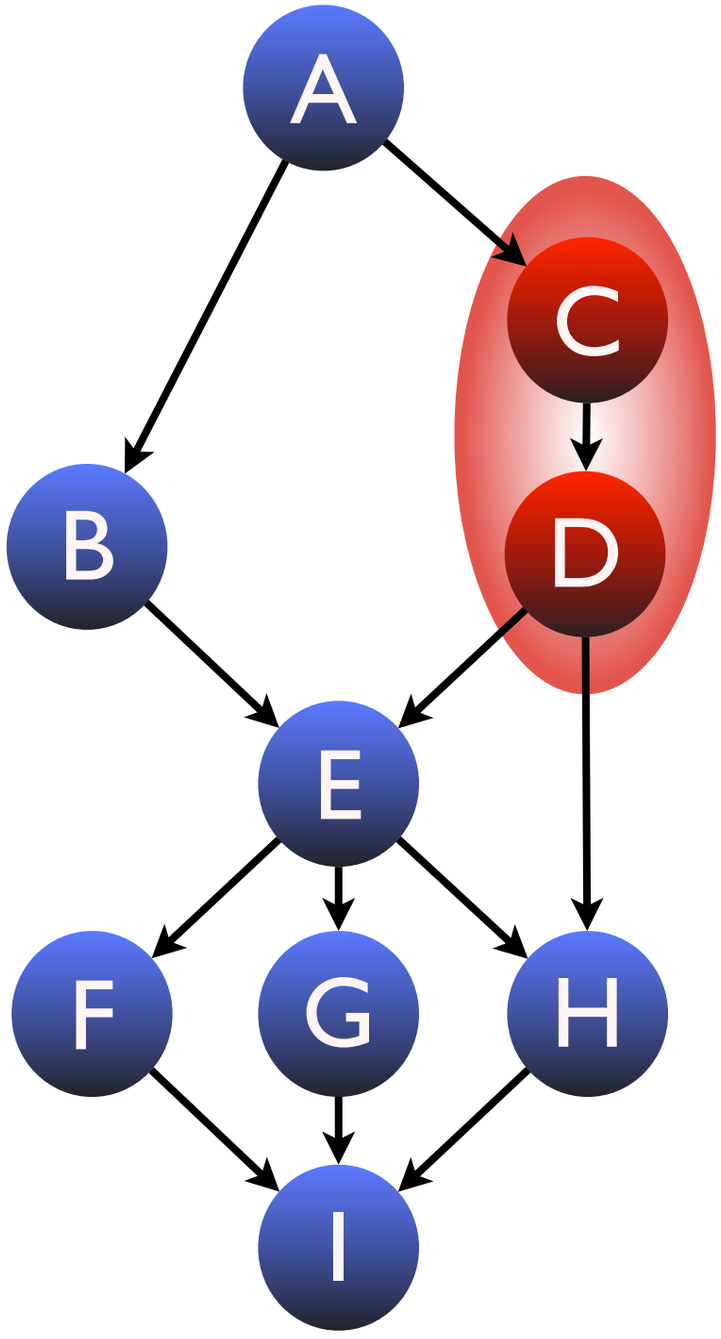
'C' and 'D' may be computed on GPU with a single copy-in/copy-out penalty.

"Graph coalescing" prevents "D" from being allocated on CPU



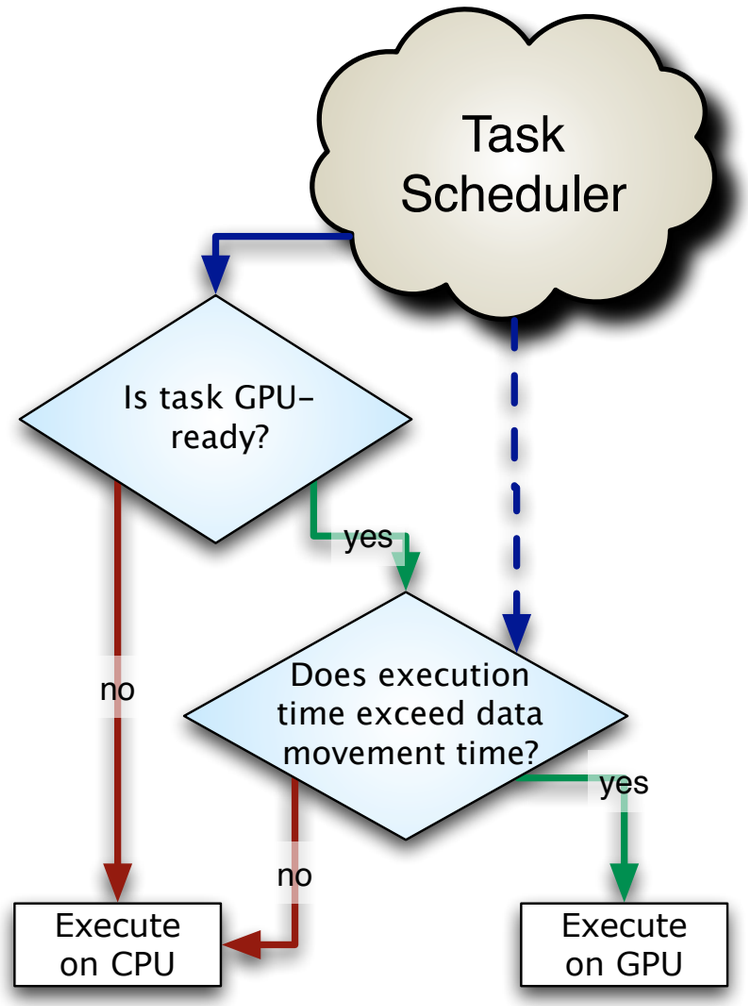
- DSL provides support for GPU deployment of operations.

Current Work - Hybrid CPU/GPU



GPU - enabled nodes

'H' may be copied while 'E' is computing, thereby hiding some latency.



- DSL provides support for GPU deployment of operations.
- Graph provides optimal scheduling of tasks across the heterogeneous system.
- Need many of tasks with lots of work (data parallel) in each.

Conclusions

- Multiple levels of parallelism will be required
- Task-based approaches can provide a great deal of insight into the structure of the problem
  - advanced memory management
  - automatic task-parallelism
  - “optimal” task scheduling in hybrid compute environments
- DSLs can simplify life (a lot!)
  - provide high-level interface to express intent, dispatch through highly optimized back-ends tuned to an architecture.
  - Programmer need not worry about architecture details, or data layout details.
  - C++ template meta programming ensures robust (correct) code.
  - Write more robust, efficient code in shorter time.
  - revise DSL back-end to affect changes through the entire code base.