Liszt

Programming Mesh-based PDE Solvers
for
Heterogeneous Parallel Platforms

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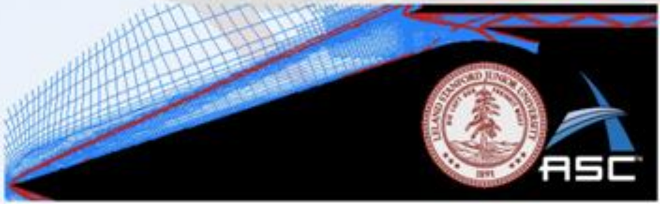


Today:

Compiling code for parallel machines

Language design that enables code compilation for parallel mach

- Abstracting away machine details
- Inferring data accesses

Implementing transformations and analysis

- Abstract analysis at compile time
- Build concrete data structures at runtime

Running code on different parallel machines

- Partitioning, Coloring
- Using analyses to target these approaches

The Future is Now

LANL IBM Roadrunner

(Opteron + Cell)

Tianhe-1A

(Xeon + Tesla M2050)

ORNL Titan

Why?

1. Specialization leads to efficiency (performance/Watt)
   - Sequential cores optimized for hiding latency
   - Throughput cores optimized for delivering FLOPs
   - Special hardware for compression-decompression, etc.
   - Laptops need to run graphics applications

2. Hybrid architectures more efficient for complex workloads
   - Applications have both task- and data-parallelism
   - Optimal platform has mixture of optimized units
   - Modern version of Amdahl’s Law

Different Technologies at Different Scales

Cluster of SMPs – racks

- Distributed memory over system area network

Small number of CMPs – boards

- Shared memory using chip interconnect

CMP - chips

- Multi-core for sequential performance
- Many-core for throughput performance
- On-chip network

Naturally Different Programming Models

Cluster of SMPs – racks

- *Message passing - MPI*

Small number of Hybrid CMPs – boards

- *Threads and locks – pthreads, OpenMP*

Hybrid CMP – chips

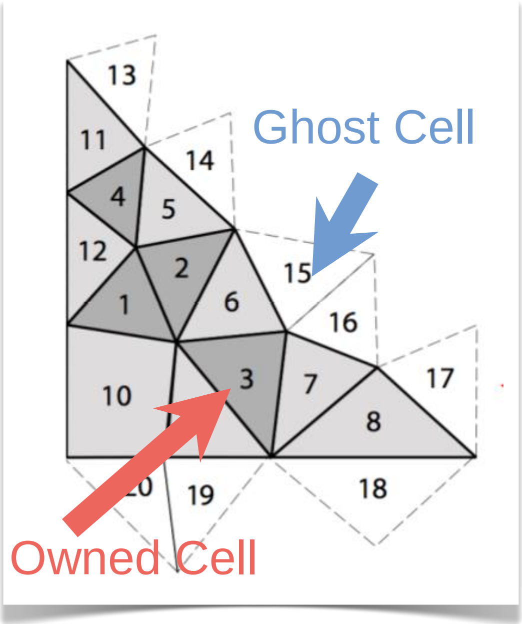
- *GPU cores – CUDA/OpenCL?*
- *Cores with vector instructions – ArBB??*
- *Task queues for scheduling work between CPU/GPU - Gramps???*

How Do We Execute on These Machines?

Execution Strategies

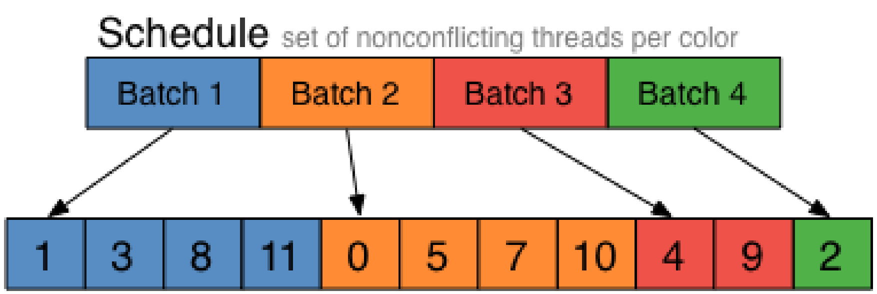
Partitioning

- Assign partition to each computational unit
- Use ghost elements to coordinate cross-boundary communication.
- Ideal for single computational unit per memory space



Coloring

- Calculate interference between work items on domain
- Schedule work-items into non-interfering batches
- Ideal for many computational units per memory space



How Do We Program These Machines?

Let the compiler help us.

Compiling to parallel computers

Find Parallelism

Expose Data Locality

Reason about Synchronization

Analyzing data dependencies

"What data does this value depend on"

Find Parallelism

- Independent data can be computed in parallel

Expose Data Locality

- Partition based on dependency

Reason about Synchronization

- Don't compute until the dependent values are known

What does avg[i] depend on?

```
int num_id = count_idx();
int* id = read_idx();
int* value = read_values();
int* data = read_data();
int* avg = malloc(num_id * sizeof(int))

for (int i = 0; i < num_id; i++) {
    for (int j = id[i]; j < id[i+1]; j++) {
        avg[i] += data[j];
    }
}
```

Can’t be done by compilers <u>in general</u>!

A[i] = B[f(i)] – must compute f(i) to find dependency

What does avg[cell] depend on?

```
int num_id = count_idx();
int* id = read_idx();
int* value = read_values();
int* data = read_data();
int* avg = malloc(num_id * sizeof(int))

for (cell <- cells(mesh)) {
    for (vertex <- vertices(cell)) {
        avg[cell] += data[vertex];
    }
}
```

Avg[cell] depends on data[] for all vertices connected to this cell. We assume this will be a small subset of data[]. Encode this!

Trade off generality
EDSLs solve the dependency problem

Liszt provides domain specific language features to solve the dependency problem:

- Parallelism
- Data Locality
- Synchronization

For solving PDEs on meshes:

All data accesses can be framed in terms of the mesh

Example: Heat Conduction on Grid

```
val Position = FieldWithLabel[Vertex,Float3](“position”)
val Temperature = FieldWithConst[Vertex,Float](0.0f)
val Flux = FieldWithConst [Vertex,Float](0.0f)
val JacobiStep = FieldWithConst[Vertex,Float](0.0f)
var i = 0;
while (i < 1000) {
  for (e <- edges(mesh)) {
    val v1 = head(e)
    val v2 = tail(e)
    val dP = Position(v1) - Position(v2)
    val dT = Temperature(v1) - Temperature(v2)
    val step = 1.0f/(length(dP))
    Flux(v1) += dT*step
    Flux(v2) -= dT*step
    JacobiStep(v1) += step
    JacobiStep(v2) += step
  }
  for (p <- vertices(mesh)) {
    Temperature(p) += 0.01f*Flux(p)/JacobiStep(p)
  }
  for (p <- vertices(mesh)) {
    Flux(p) = 0.f; JacobiStep(p) = 0.f;
  }
  i += 1
}
```

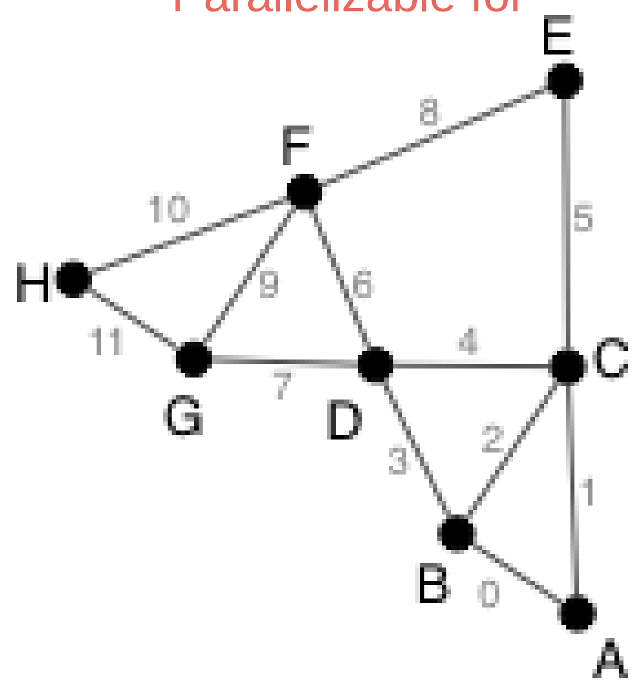
Mesh Elements

Topology Functions

Sets

Fields (Data storage)

Parallelizable for



Features of high performance PDE solvers

Find Parallelism

- Data-parallelism on mesh elements

Expose Data Locality

- PDE Operators have local support
- Stencil captures exact region of support

Reason about Synchronization

- Iterative solvers
- Read old values to calculate new values

Liszt Language Features

Mesh Elements

- Vertex, Edge, Face, Cell

Sets

- cells(mesh), edges(mesh), faces(mesh), …

Topological Relationships

- head(edge), vertices(cell), …

Fields

- val vert_position = position(v)

Parallelism

- forall statements: for(f <- faces(cell)) { … }

How do we infer data accesses from Liszt?

“Stencil” of a piece of code:

- Captures just the memory accesses it performs

Infer stencil for each for-comprehension in Liszt

Language Features for Parallelism

```
for (e <- edges(mesh)) {
    …
}
```

Data-parallel for-comprehension

- Calculations are independent
- No assumptions about how it is parallelized
- Freedom of underlying runtime implementation

Language Features for Locality

Automatically infer stencil (pattern of memory accesses at element)

Restrictions:

- Mesh elements only accessed through built-in topological functions; cells(mesh), …
- Variable assignments to topological elements and fields are immutable; val v1 = head(e)
- Data in Fields can only be accessed using mesh elements JacobiStep(v1)
- No recursive functions

Language Features for Synchronization

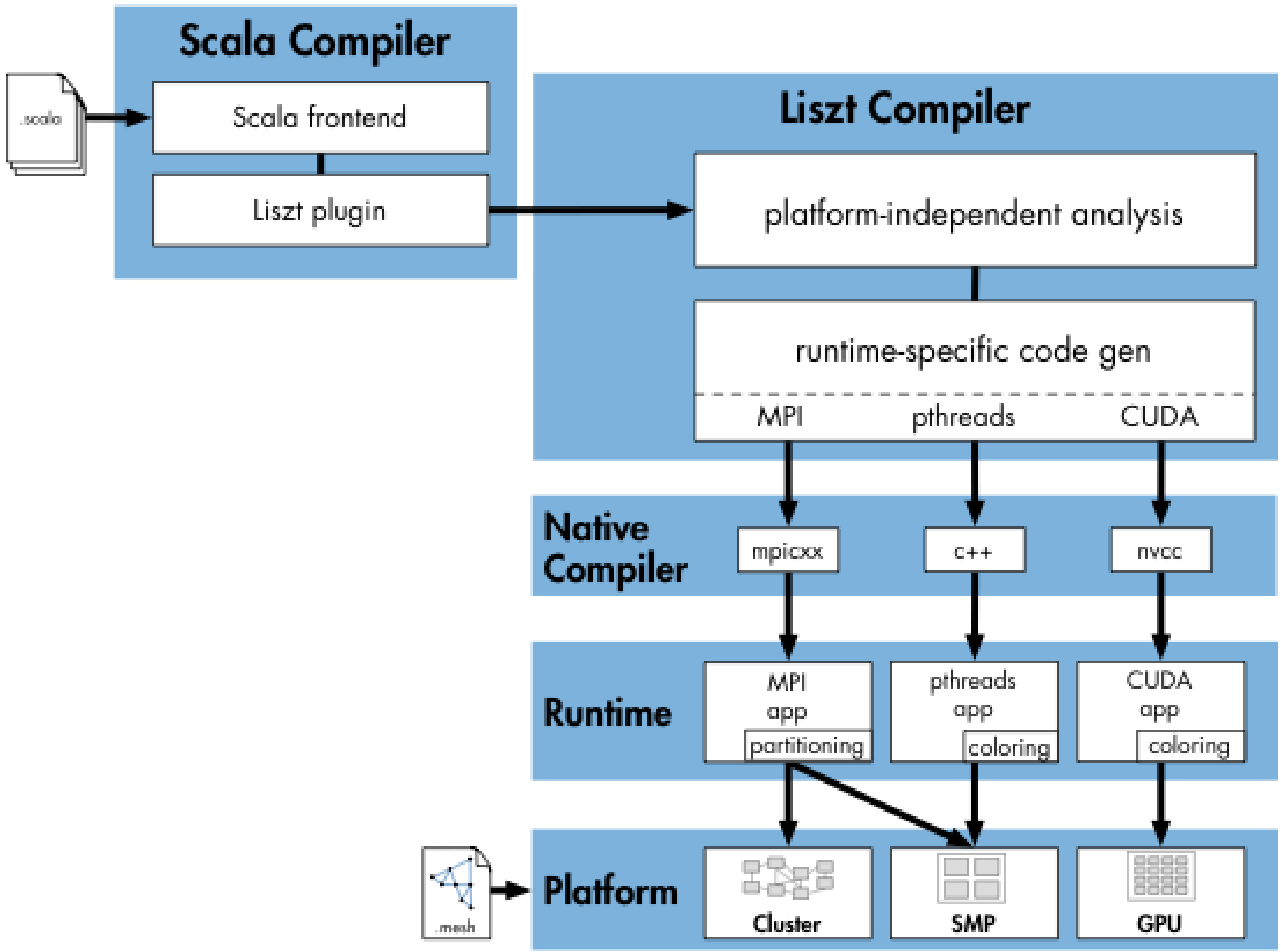
Phased usage of Fields

- Fields have *field phase* state
  - read-only, write-only, reduce-using-operator `field(el) [op]= value`
- Fields cannot change phase within for-comprehension

Associative Operators

- Allow single expensive calculation to write data to multiple elements
- Provide atomic scatter operations to fields
  - e. g. `field(el) += value`
- Introduce write dependencies between instances of for-comprehension

Architecture

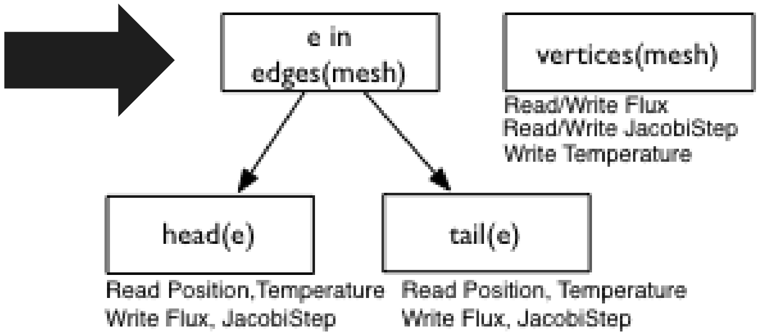


Domain Specific Transform:
Inferring Stencils through Stencil Detection

Analyze code to detect memory access stencil of each top-level for-all comprehension

- Extract nested mesh element reads
- Extract field operations
- Difficult with a traditional library

```
for (e <- edges(mesh)) {
  val v1 = head(e)
  val v2 = tail(e)
  val dP = Position(v1) - Position(v2)
  val dT = Temperature(v1) - Temperature(v2)
  val step = 1.0f/(length(dP))
  Flux(v1) += dT*step
  Flux(v2) -= dT*step
  JacobiStep(v1) += step
  JacobiStep(v2) += step
}
```



Domain Specific Transform:
Inferring Stencils through Stencil Detection

$$S(e_l, E) = (R, W)$$

e_l Expression

E Environment mapping free variables to values

$$(e_l, E) \qquad\qquad (R, W)$$

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for (e <- edges(mesh)) {
  val v1 = head(e)
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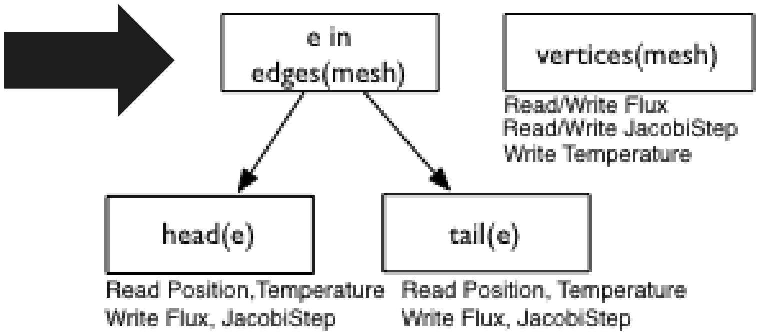

Domain Specific Transform:
Inferring Stencils through Stencil Detection

Problem: Don't know the mesh at compile time!

Break up inference into:

Static part: Abstractly reason about operators.

generate c++ code that queries mesh to build the specific stencil for each for-comprehension

Dynamic part: Concretely build data structures by analyzing mesh

run c++ code on mesh

Anything that directly depends on mesh becomes generated code, executed at runtime.

This means: It is possible to write low-level c++ code that targets our back-end. But ugly and hard!

Implementing stencil detection
The way that won't work

$$S(e_l, E) = (R, W)$$

1. Sandbox code by having temporary fields and variables
2. Have every field read and write log the current stack of mesh elements
3. Run the code!

Cannot guarantee termination

Can run very long

Must do all the math beforehand. In single core.

```
for (e <- edges(mesh)) {
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  val dP = Position(v1) - Position(v2)
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  val step = 1.0f/(length(dP))
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}
```

Implementing stencil detection
Abstract Interpretation

"Partial execution of a computer program to gain insight into it's semantics". Allows us to calculate an **approximate** stencil

Apply transformation $\mathcal{T}$ to Liszt code

generate code with desirable properties (terminates, fast)

Implementing stencil detection
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$$S(e_l, E) \subseteq \bar{S}(e_l, E) = (R, W)$$

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  JacobiStep(v1) += step
  JacobiStep(v2) += step
}
```

$\mathcal{T}$

```
for (e <- edges(mesh)) {
  val v1 = head(e)
  val v2 = tail(e)
  val dP = Position(v1) - Position(v2)
  val dT = Temperature(v1) - Temperature(v2)

  Flux(v1) += _
  Flux(v2) -= _
  JacobiStep(v1) += _
  JacobiStep(v2) += _
}
```

Implementing stencil detection
Abstract Interpretation

Defining $\mathcal{T}$

$$\mathcal{T}(\ \text{if}(e_p)\ e_t\ \text{else}\ e_e\ ) = \ \mathcal{T}(e_p); \mathcal{T}(e_t); \mathcal{T}(e_e);$$

Conservatively evaluate if-statements

$$\mathcal{T}(\ \text{while}(e_p)\ e_b\ ) = \ \mathcal{T}(e_p); \mathcal{T}(e_b);$$

Single Static Assignment of Mesh Variables

$$\mathcal{T}(\ f(a_0,\dots,a_n)\ ) = \ f'(\mathcal{T}(a_0),\dots,\mathcal{T}(a_n))$$

Recursively apply to functions

Everything else, recursively apply to subexpressions of expression

In pictures

Domain Specific Transform:
Stencil Detection

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for (e <- edges(mesh)) {
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  Flux(v1) += _
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...
```

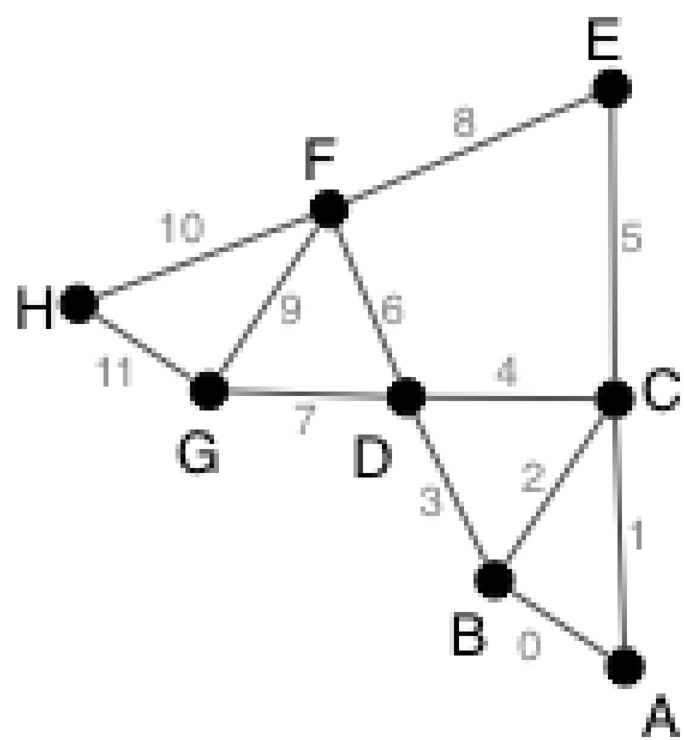

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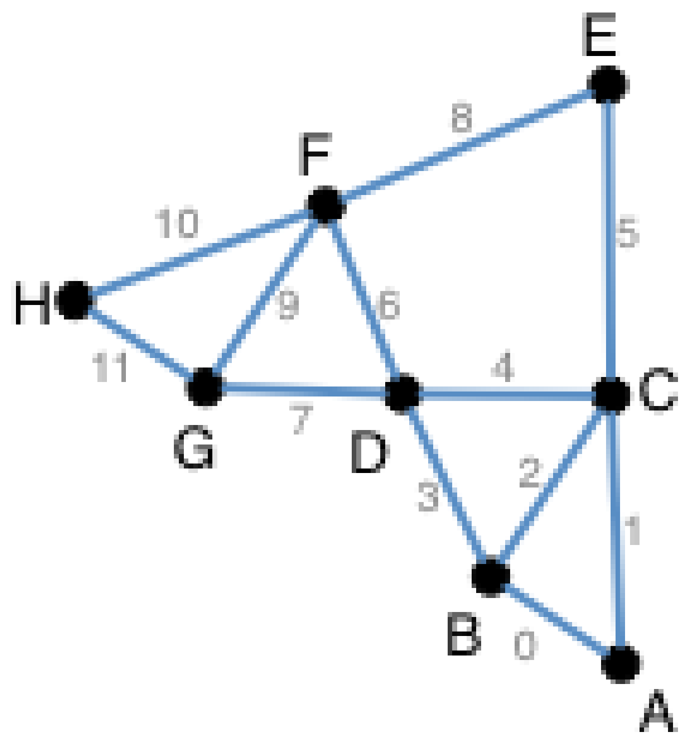
```

e in edges(mesh)



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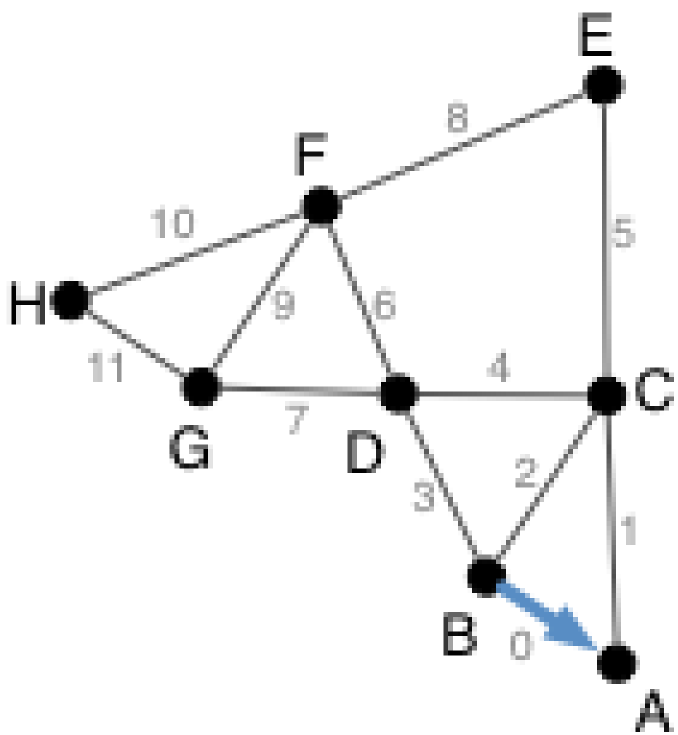

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...
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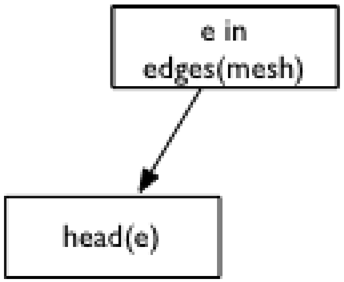

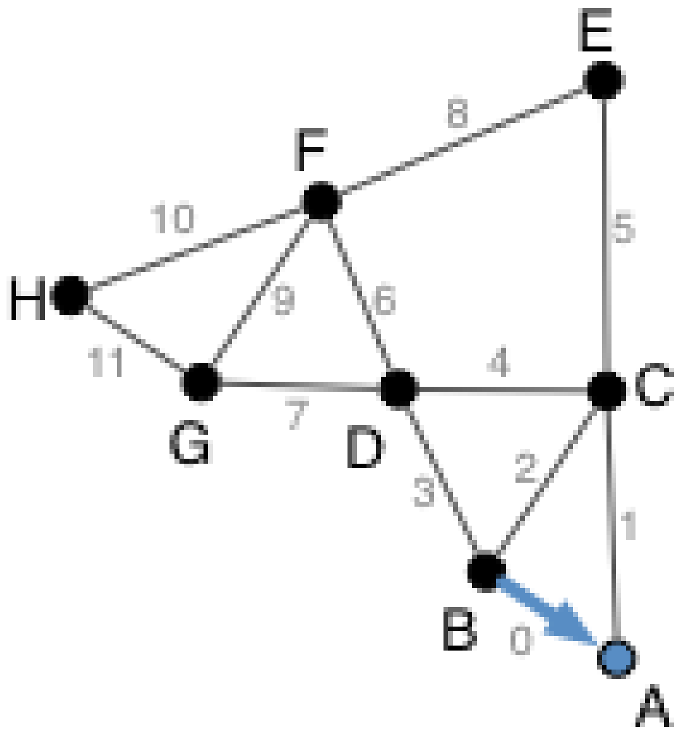

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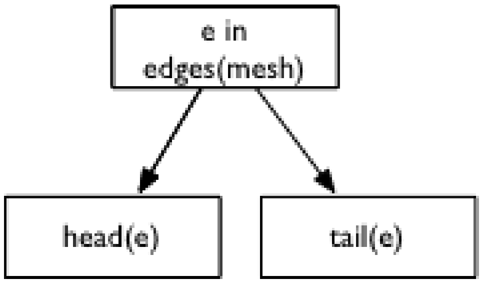

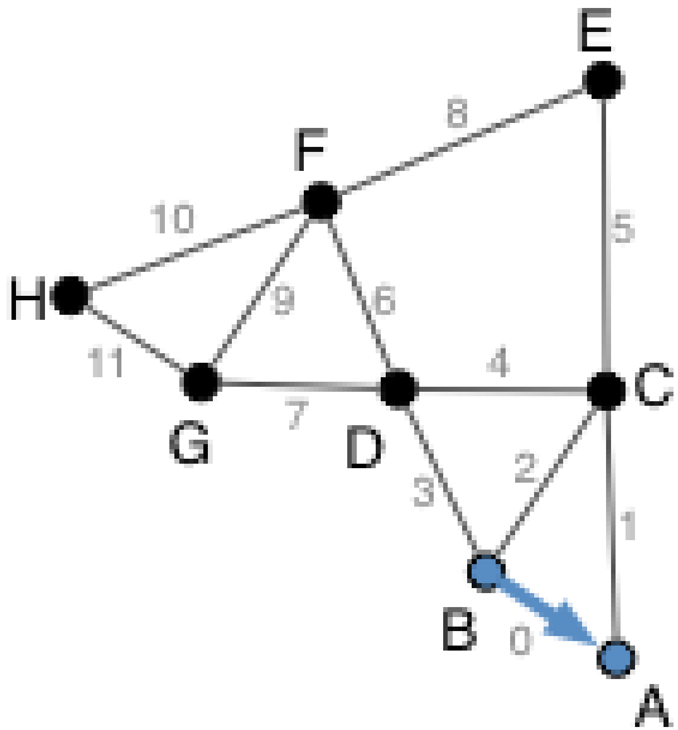

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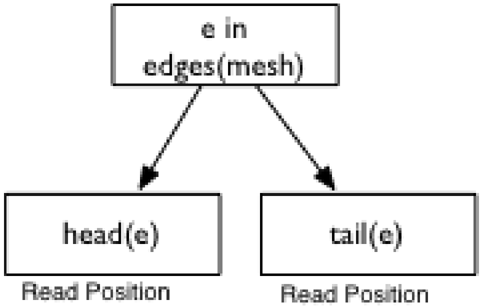

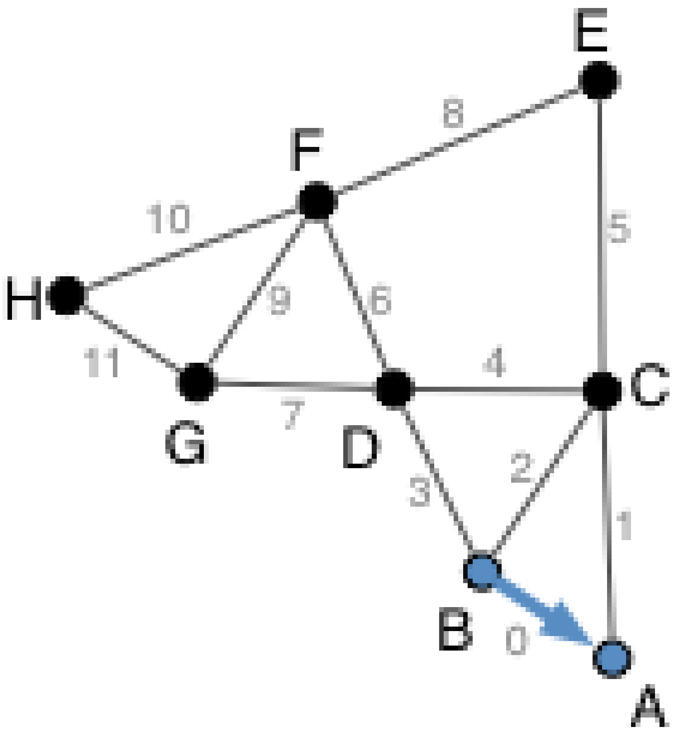

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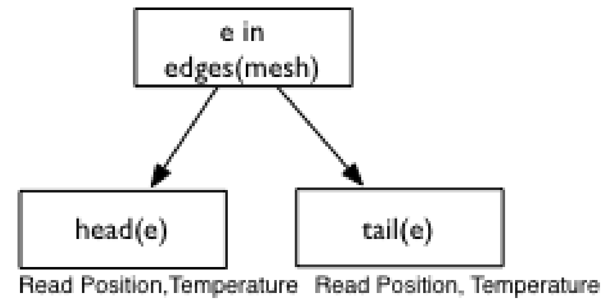

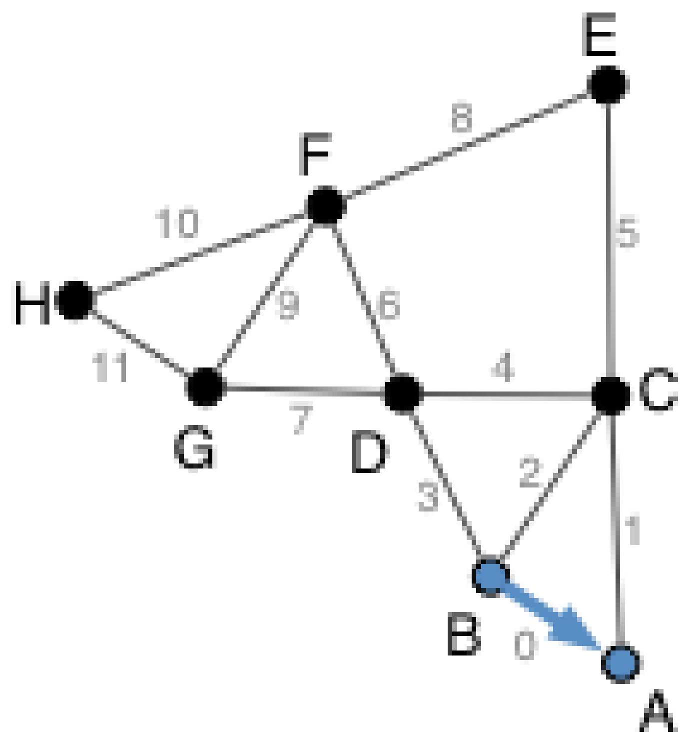

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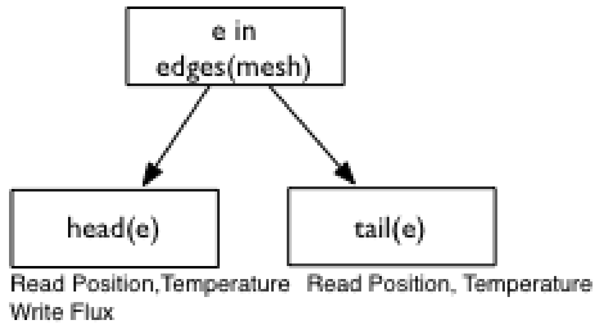

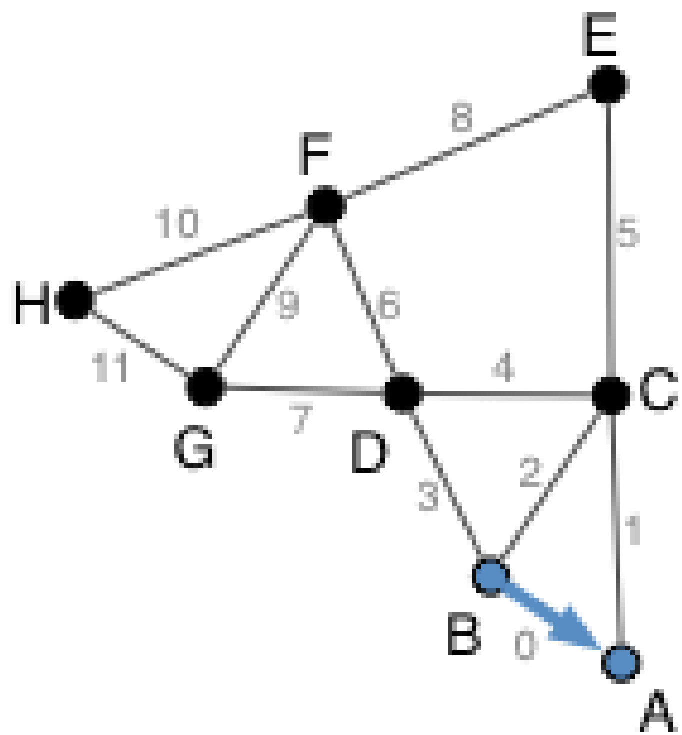

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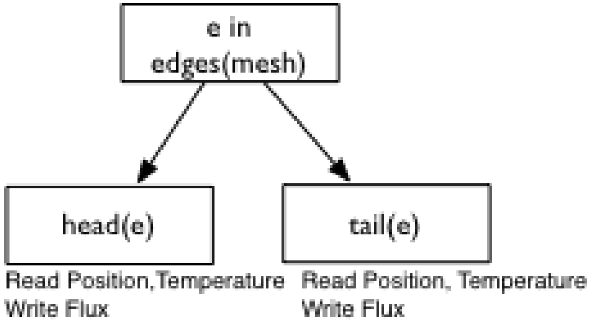

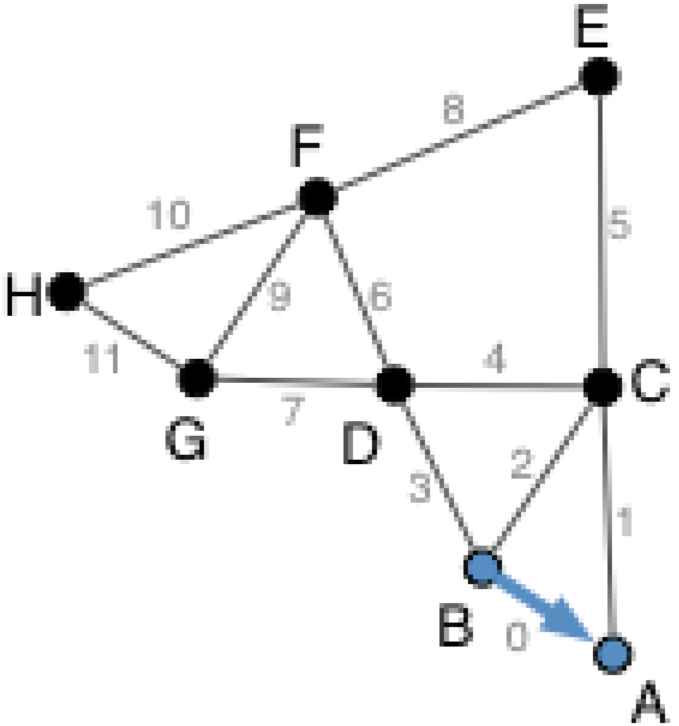

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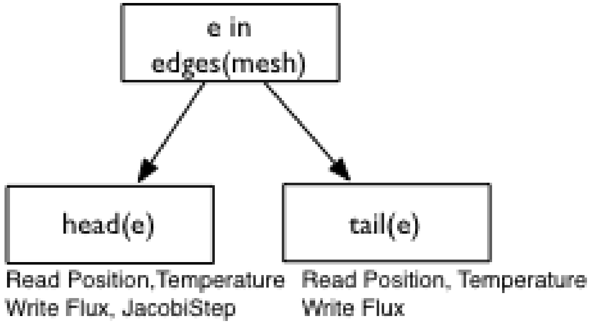

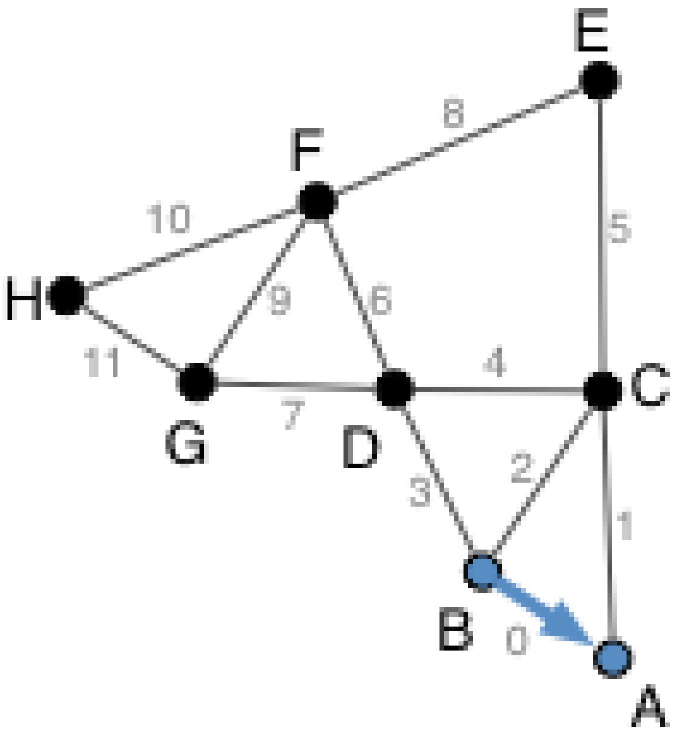

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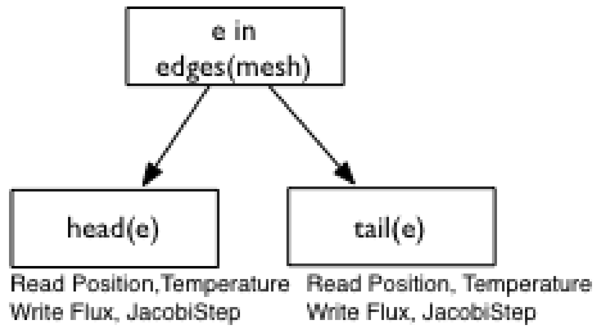

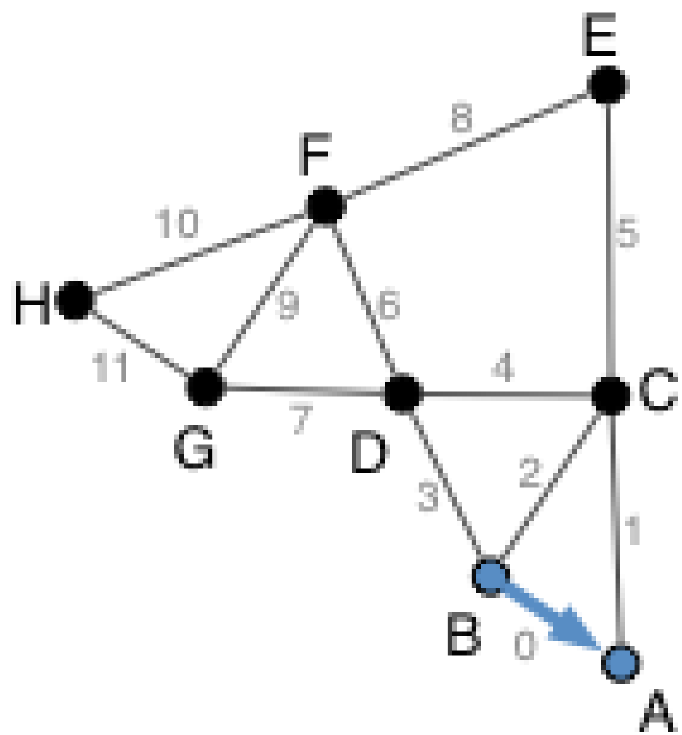

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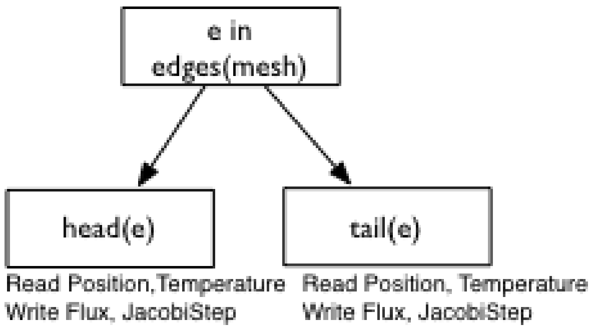

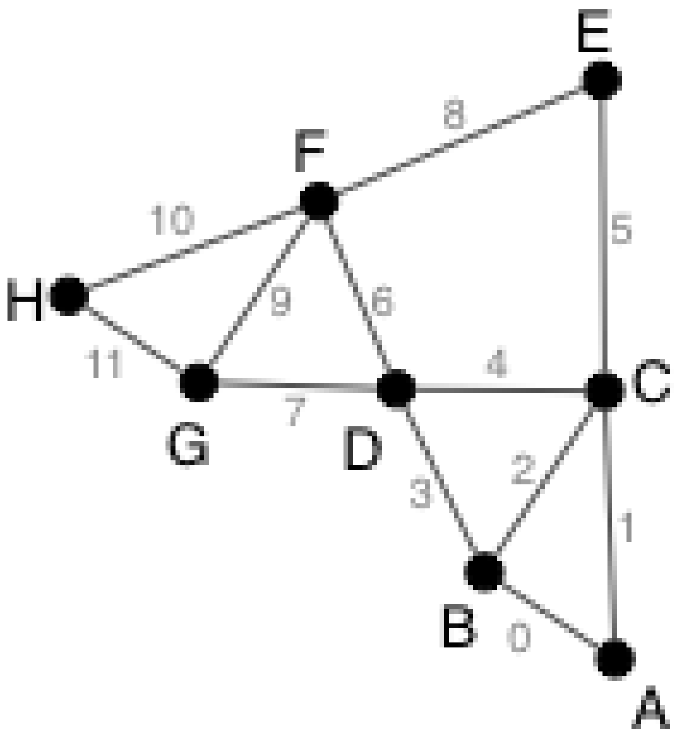

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}
```
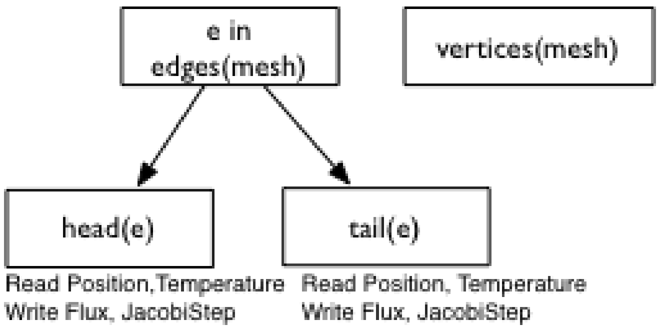
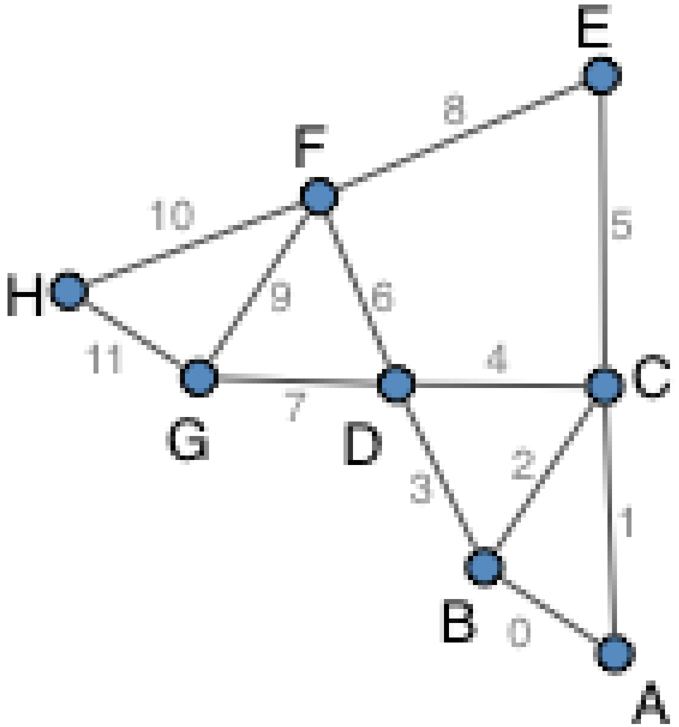
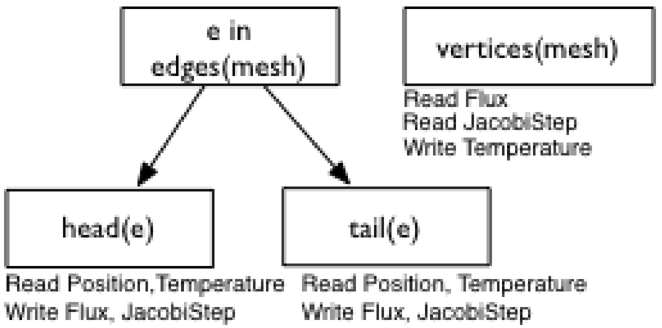
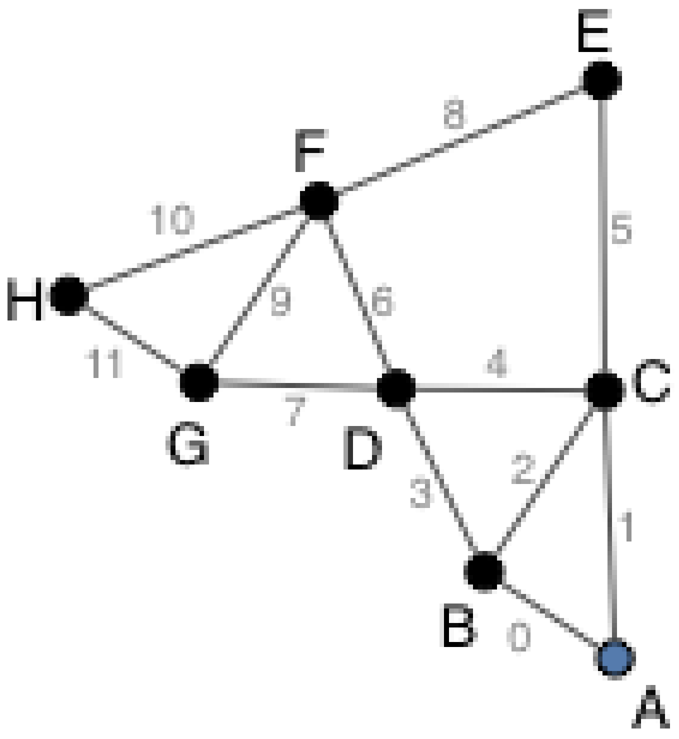





Domain Specific Transform:
Stencil Detection

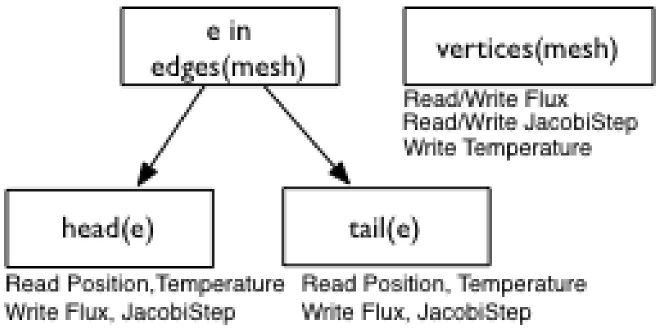
```
for (p <- vertices(mesh)) {
  Temperature(p) += Flux(p)/JacobiStep(p)
}
for (p <- vertices(mesh)) {
  Flux(p) = 0.f; JacobiStep(p) = 0.f;
}
```

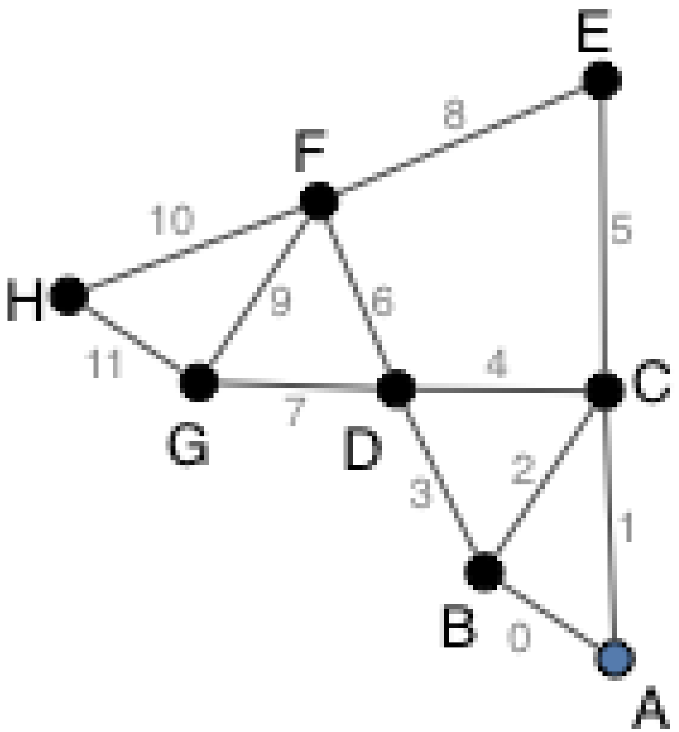




Domain Specific Transform: Stencil Detection

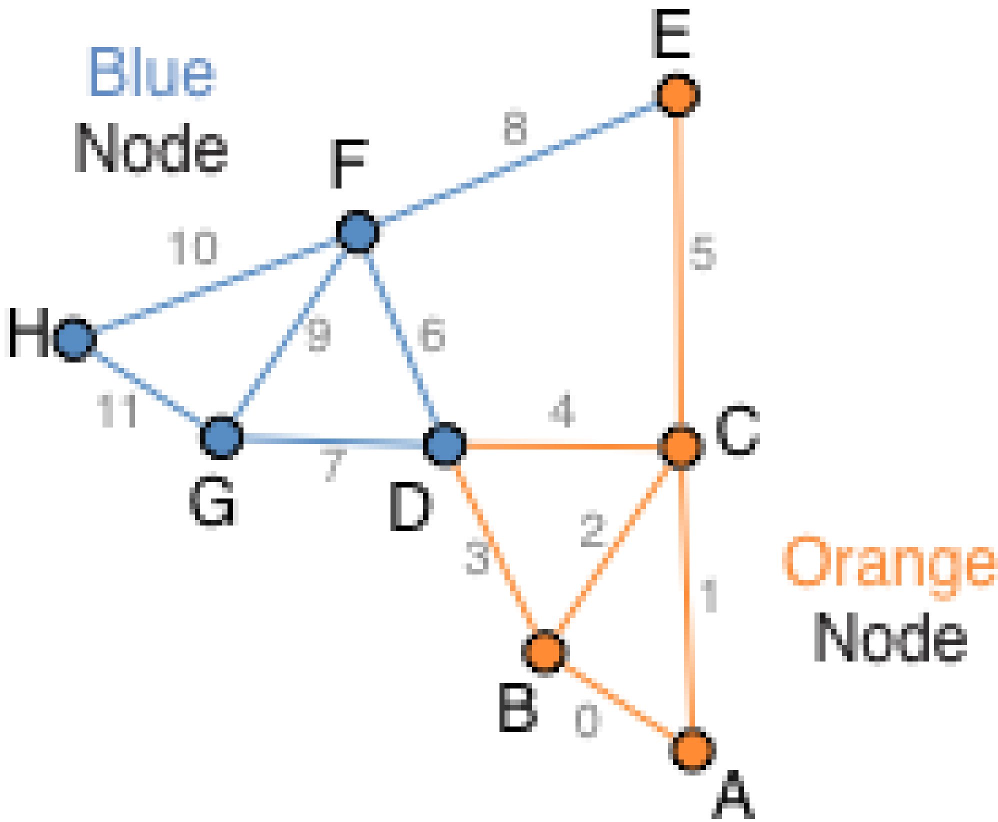
```
for (p <- vertices(mesh)) {
  Temperature(p) += 0.01f*Flux(p)/JacobiStep(p)
}
for (p <- vertices(mesh)) {
  Flux(p) = _; JacobiStep(p) = _;
}
```





MPI: Partitioning with Ghosts

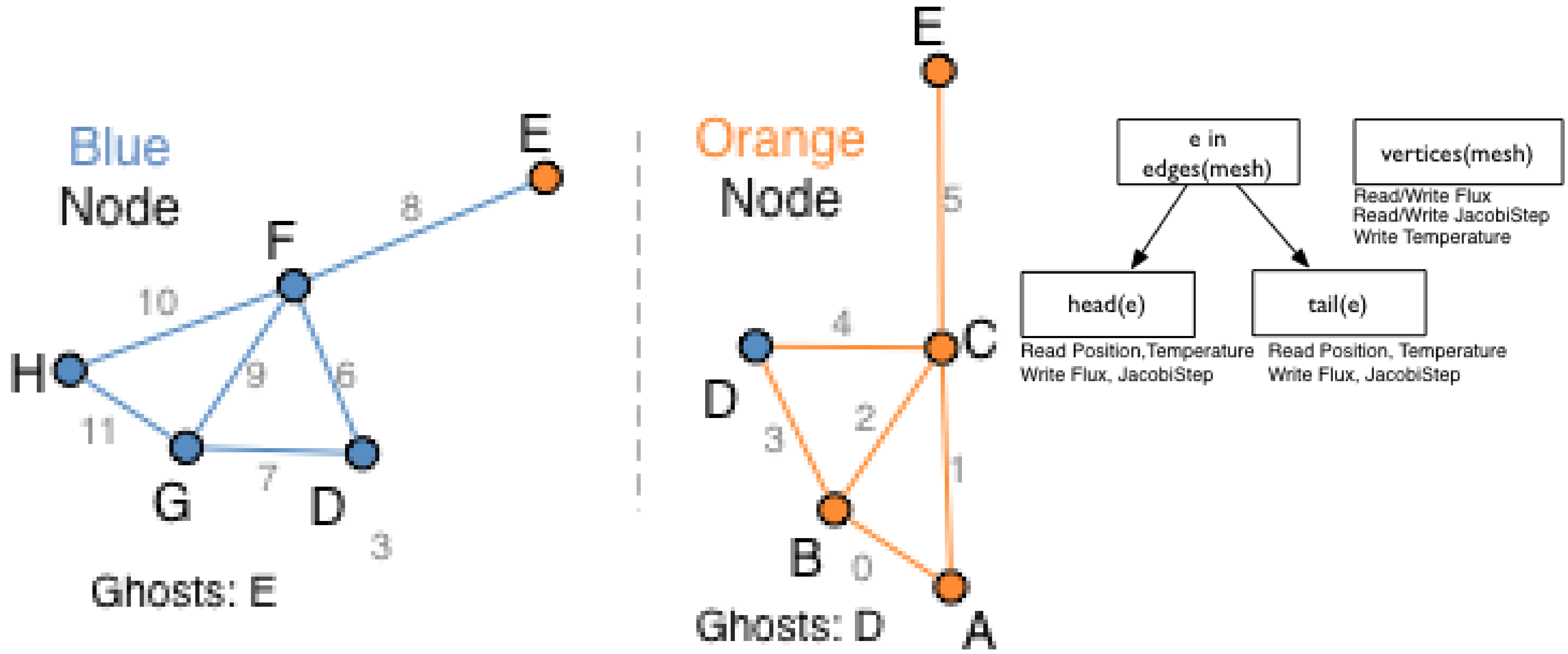
1. Partition Mesh (ParMETIS, G. Karypis)



MPI: Partitioning with Ghosts

2. Find used mesh elements and field entries using stencil data and duplicate locally into “ghost” elements

Implementation directly depends on algorithm’s access patterns



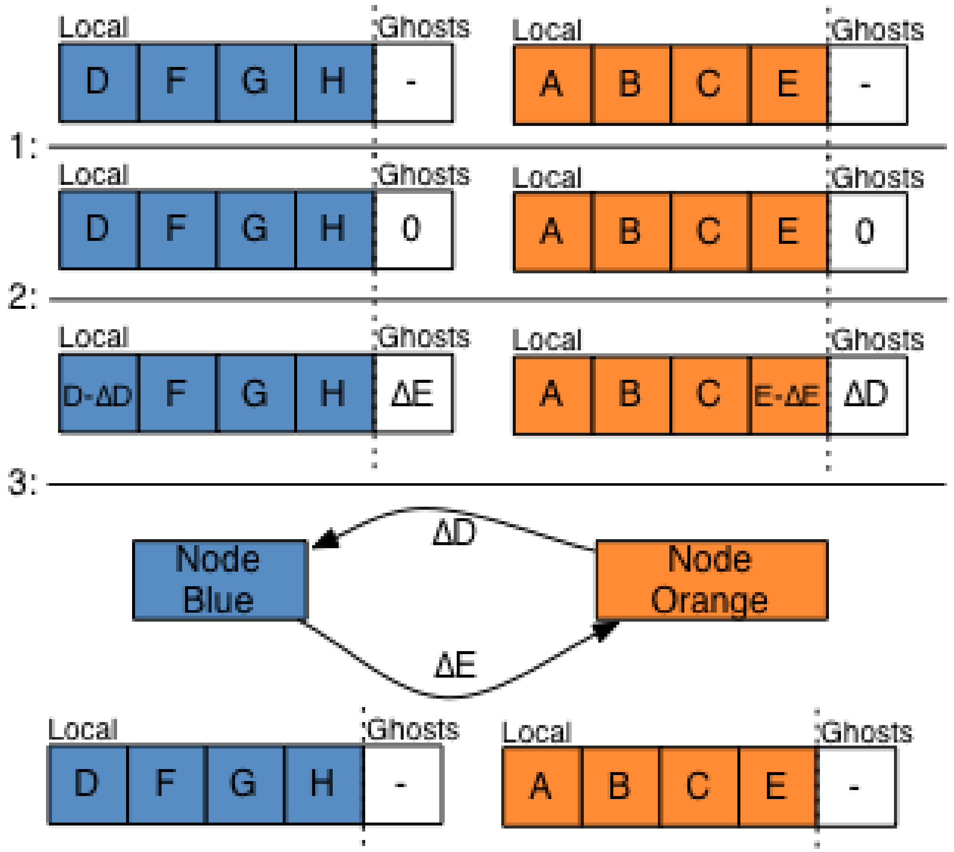
MPI: Partitioning with Ghosts

3. Annotate for-comprehensions with field preparation statements

```
Flux.ensureState<LISZT_SUM>();
JacobiStep.ensureState<LISZT_SUM>();
Position.ensureState<LISZT_READ>();
Temperature.ensureState<LISZT_READ>();
for (e <- edges(mesh)) {
    val dP = Position(v1) - Position(v2)
    ...
    Flux(v1) += dT*step
    JacobiStep(v1) += step
}
Temperature.ensureState<LISZT_SUM>();
Flux.ensureState<LISZT_READ>();
JacobiStep.ensureState<LISZT_READ>();
for (p <- vertices(mesh)) {
    Temperature(p) += 0.01f * Flux(p)/JacobiStep(p)
}
…
```

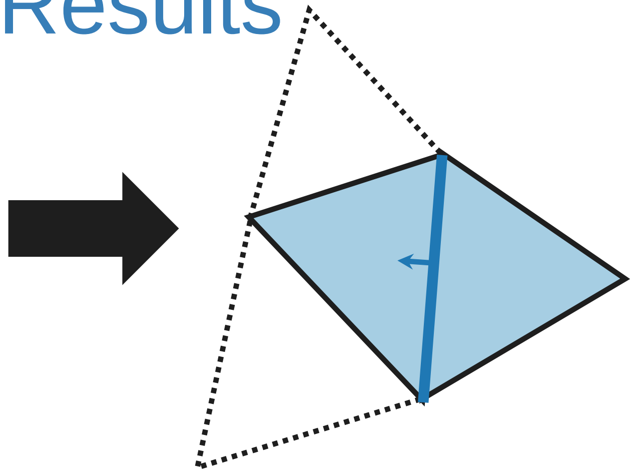
MPI: Partitioning with Ghosts

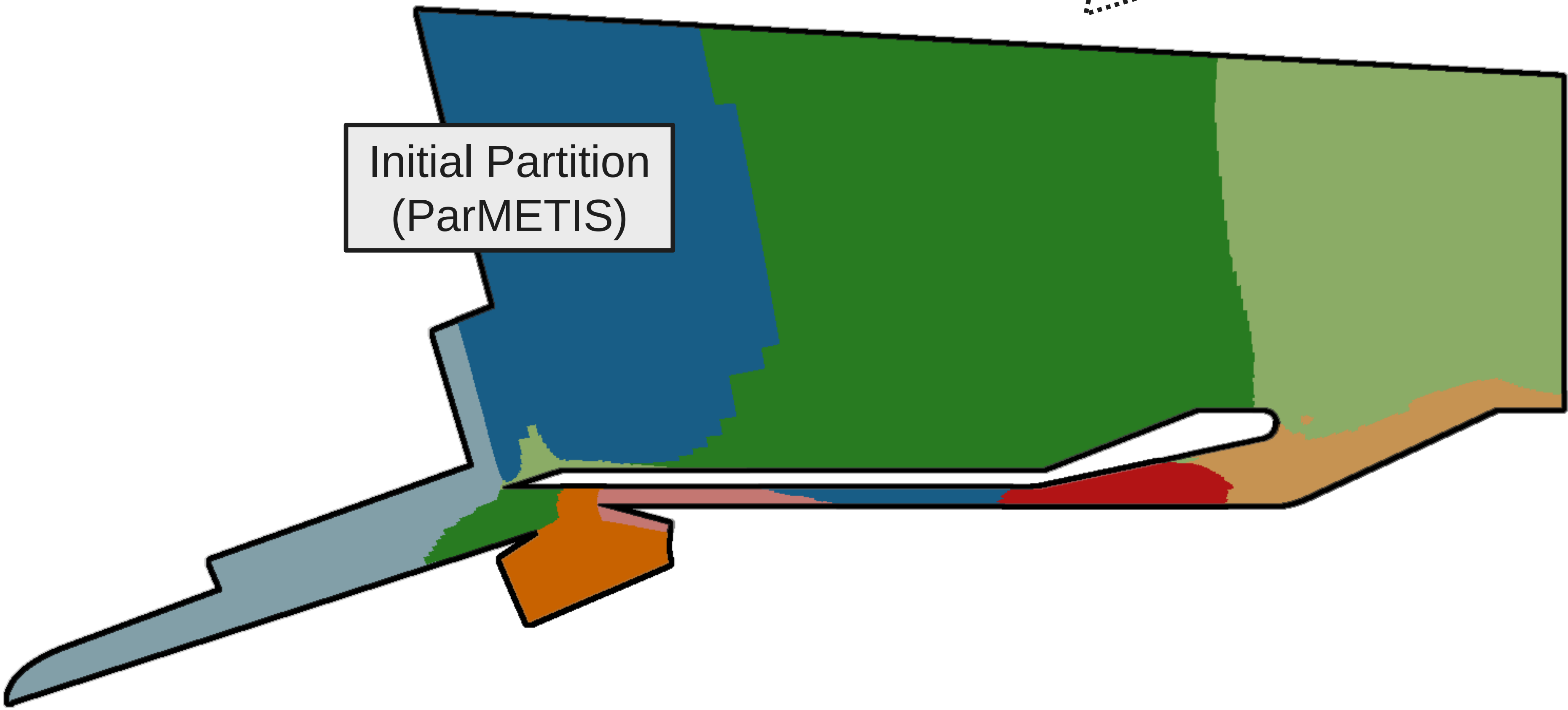
4. MPI communication is batched during for-comprehensions and only transferred when necessary



Applying Program Analysis: Results

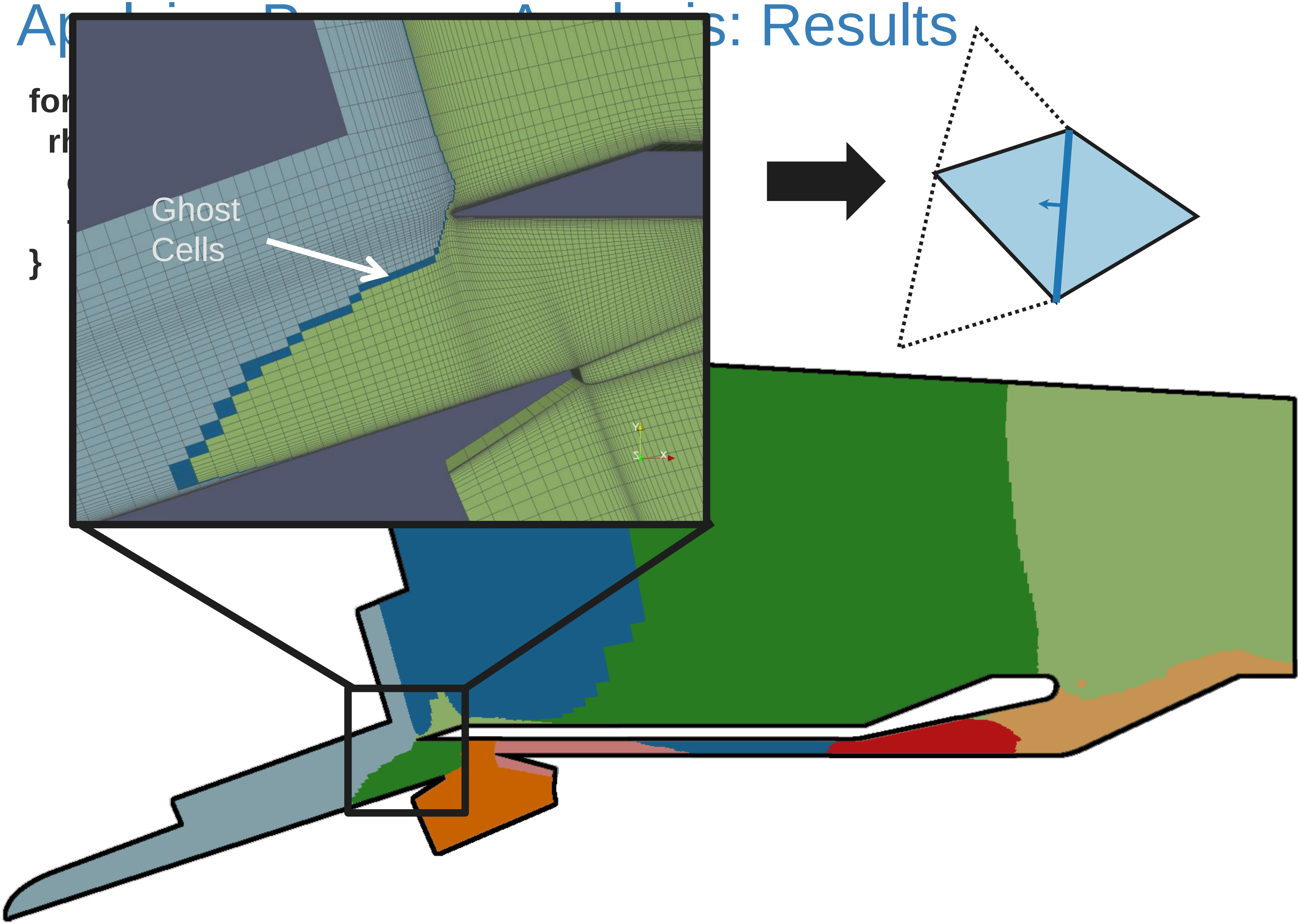
```
for(f <- faces(mesh)) {
  rhoOutside(f) :=
    calc_flux( f,rho(outside(f) ))
    + calc_flux( f,rho(inside(f) ))
}
```





Ap s: Results

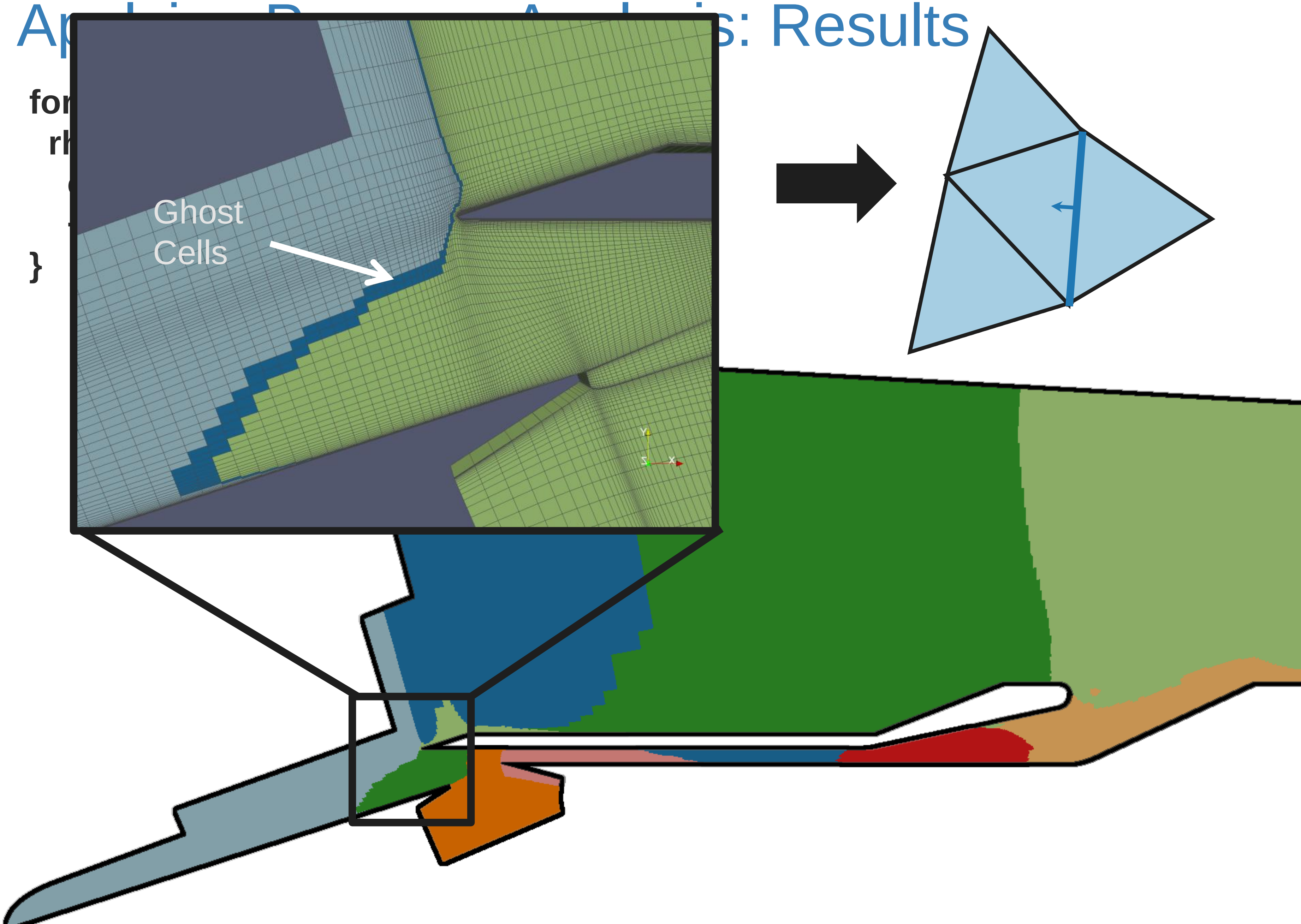
```
for
  rh
}
```



Ap s: Results

for
rh

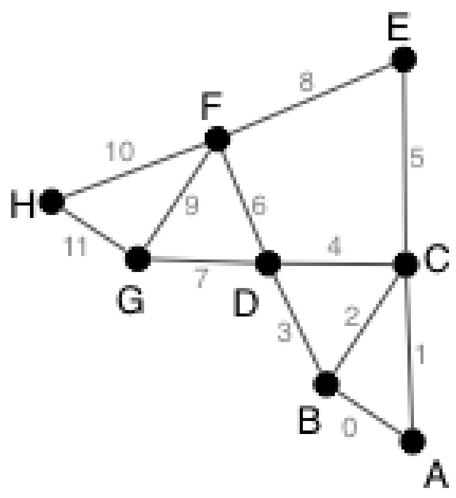
}



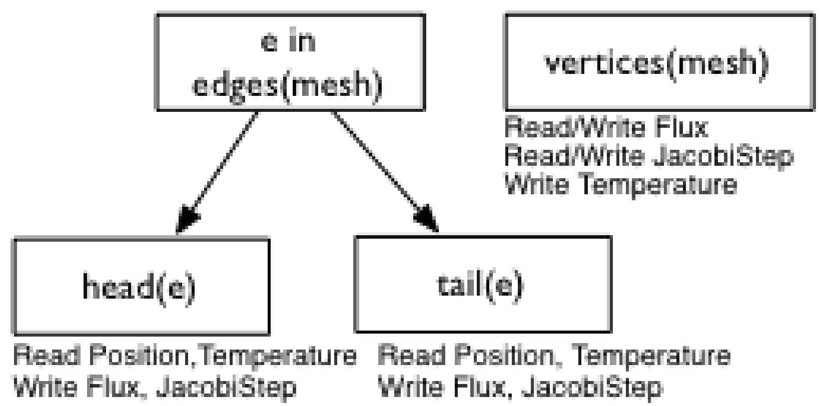
GPU: Schedule threads with coloring

- Shared Memory
- Field updates need to be atomic
- Concerns about MPI approach – volume vs surface area

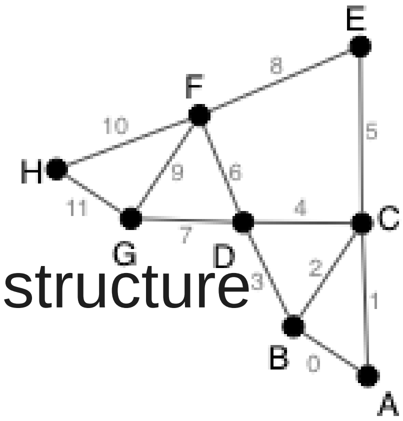
Build a graph of interfering writes:



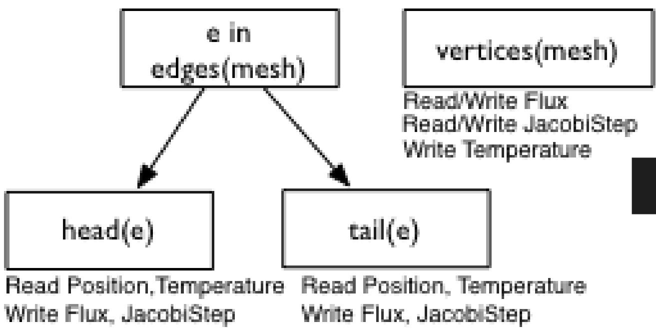
+



GPU: Schedule threads with coloring

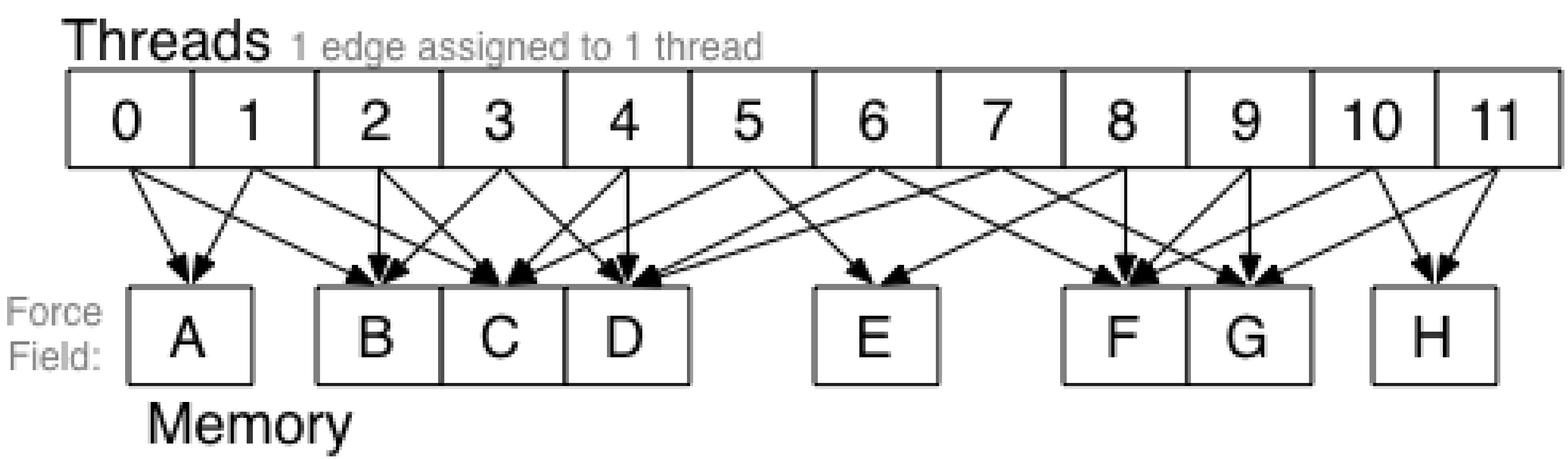


Compile time: Generate code to create field write structure

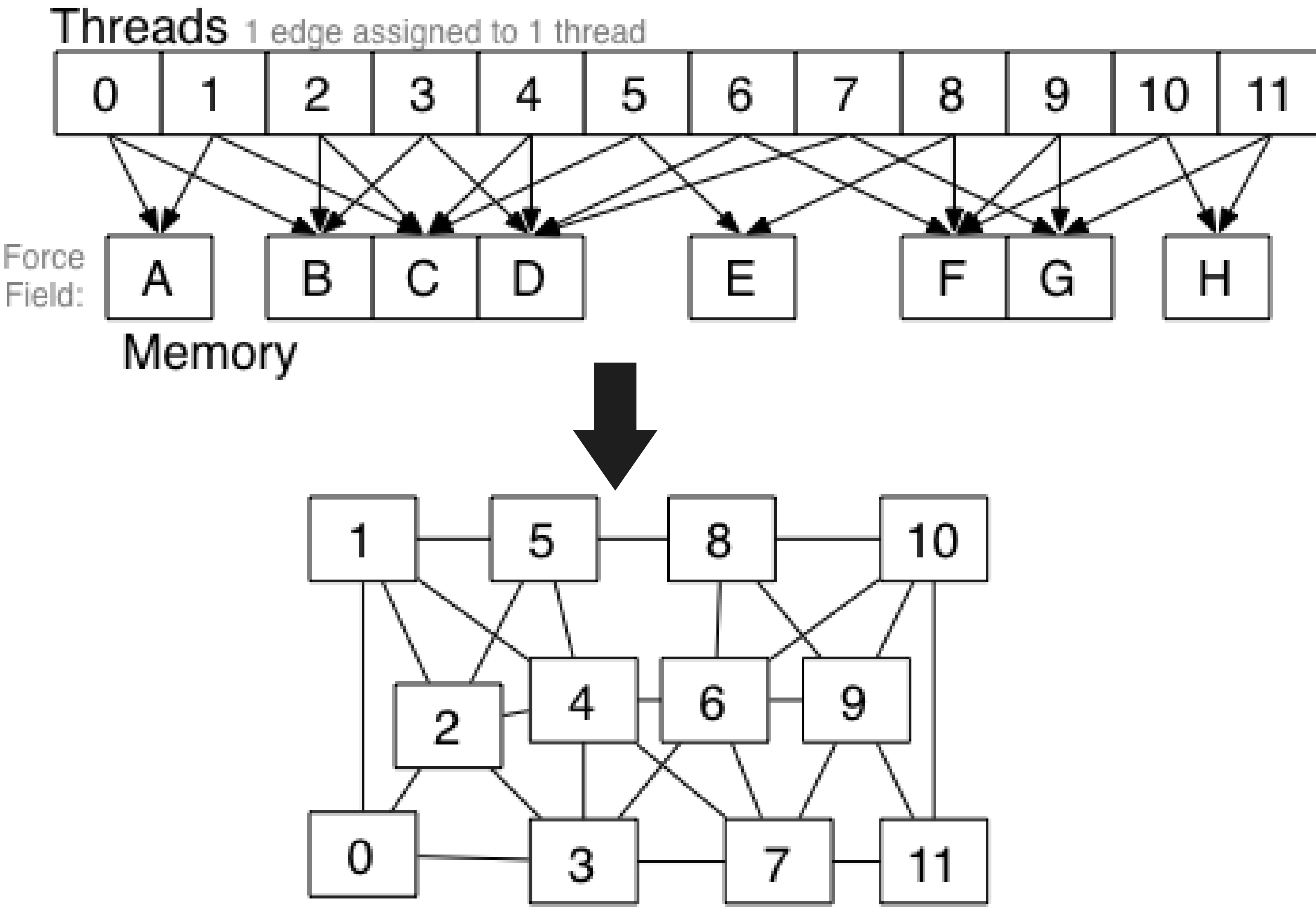



```
FORALL_SET(e,edges(mesh))
    Vertex v_1 = head(e);
    igraph->addEdge(thread(e).ID(),v_1.ID(),18886);
    Vertex v_2 = tail(e);
    igraph->addEdge(thread(e).ID(),v_12.ID(),18886);
ENDSET
```

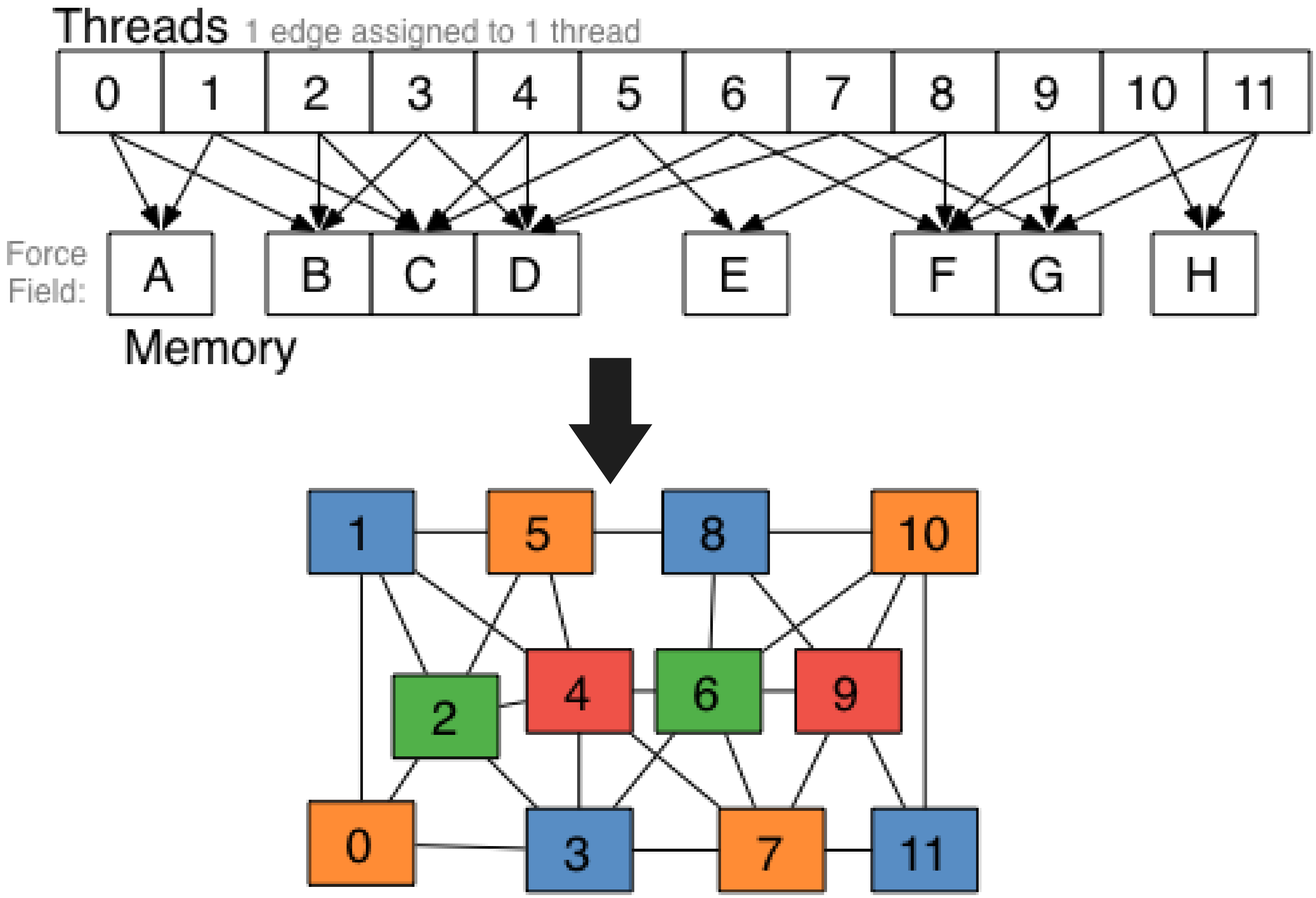
Runtime: Build this structure using mesh and stencil



GPU: Schedule threads with coloring



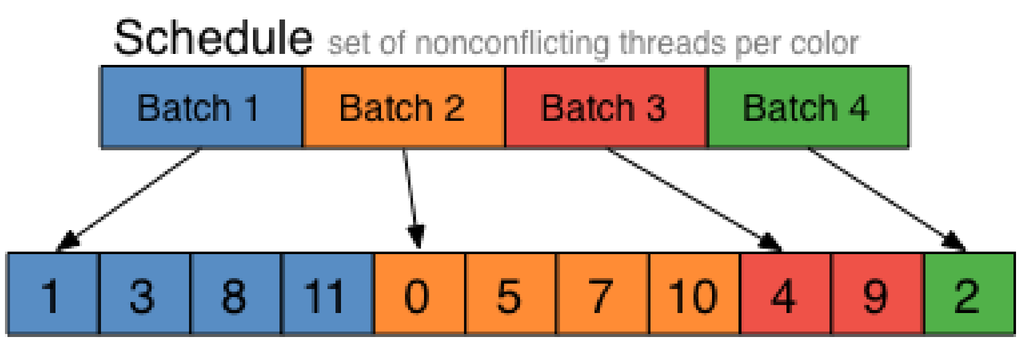
GPU: Schedule threads with coloring



GPU: Schedule threads with coloring

Convert each for-comprehension into a GPU kernel, launched multiple times for sets of non-interfering iterations.

```
__global__ for_01(ColorBatch batch, Force,
                  Position, Velocity, Maxforce) {
    val dT = Position(v1) - Position(v2)
    ...
    Flux(v1) += dT*step
    Flux(v2) -= springForce
    ….
}
WorkgroupLauncher launcher = WorkgroupLauncher_forWorkgroup(001);
ColorBatch colorBatch;
while(launcher.nextBatch(&colorBatch)) {
    Maxforce.ensureSize(colorBatch.kernel_size());
    GlobalContext_copyToGPU();
    for_01<<<batch.blocks(),batch.threads()>>>(
        batch, Force, Position,
        Velocity, Maxforce);
}
```



Results

4 example codes with Liszt and C++ implementations:

- Euler solver from Joe
- Navier-Stokes solver from Joe
- Shallow Water simulator
  - Free-surface simulation on globe as per Drake et al.
  - Second order accurate spatial scheme
- Linear FEM
  - Hexahedral mesh
  - Trilinear basis functions with support at vertices
  - CG solver

Scalar Performance Comparisons

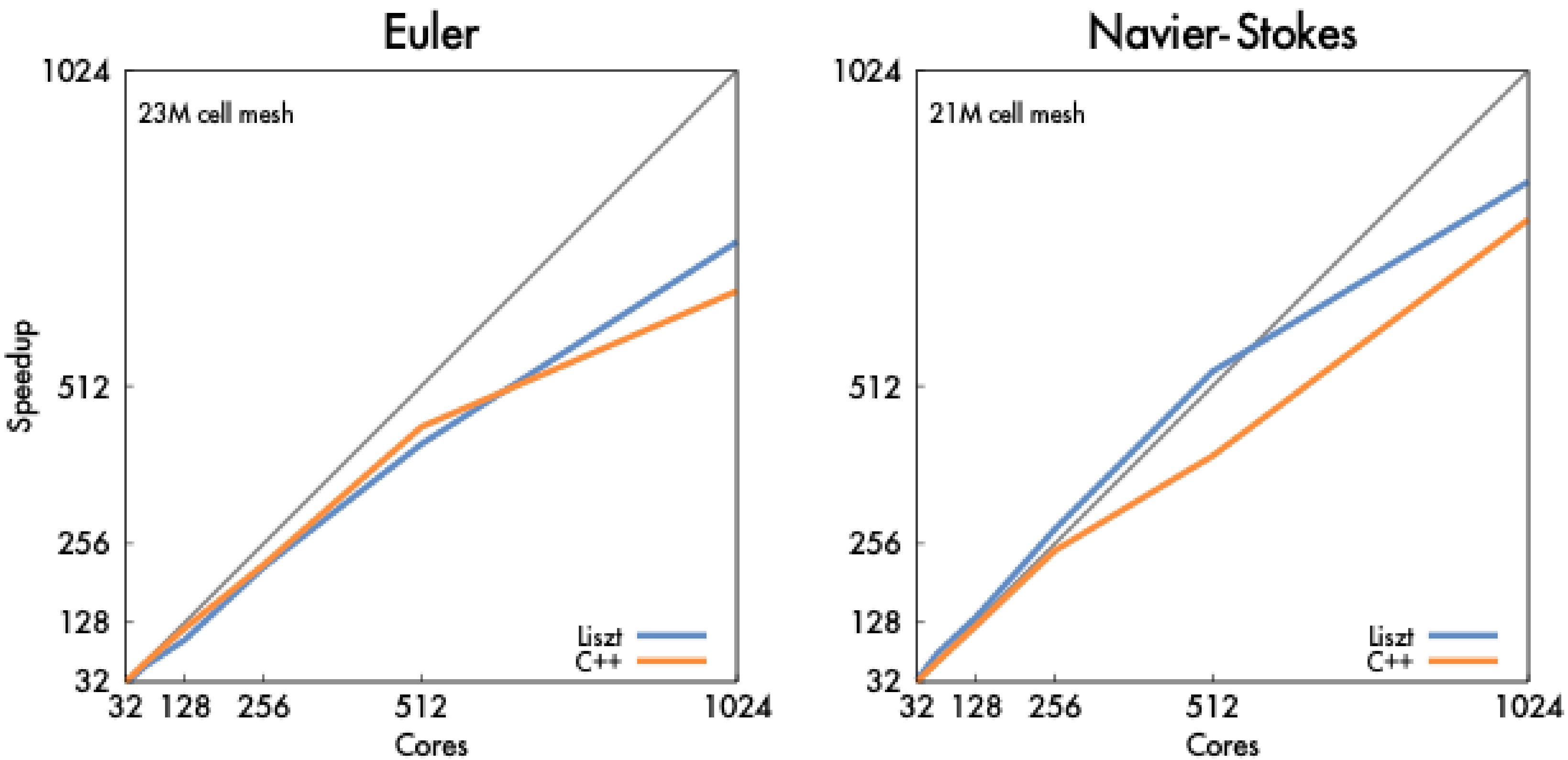
Runtime comparisons between hand-tuned C++ and Liszt

Liszt performance within 12% of C++

	Euler	Navier-Stokes	FEM	Shallow Water
Mesh size	367k	668k	216k	327k
Liszt	0.37s	1.31s	0.22s	3.30s
C++	0.39s	1.55s	0.19s	3.34s

MPI Performance

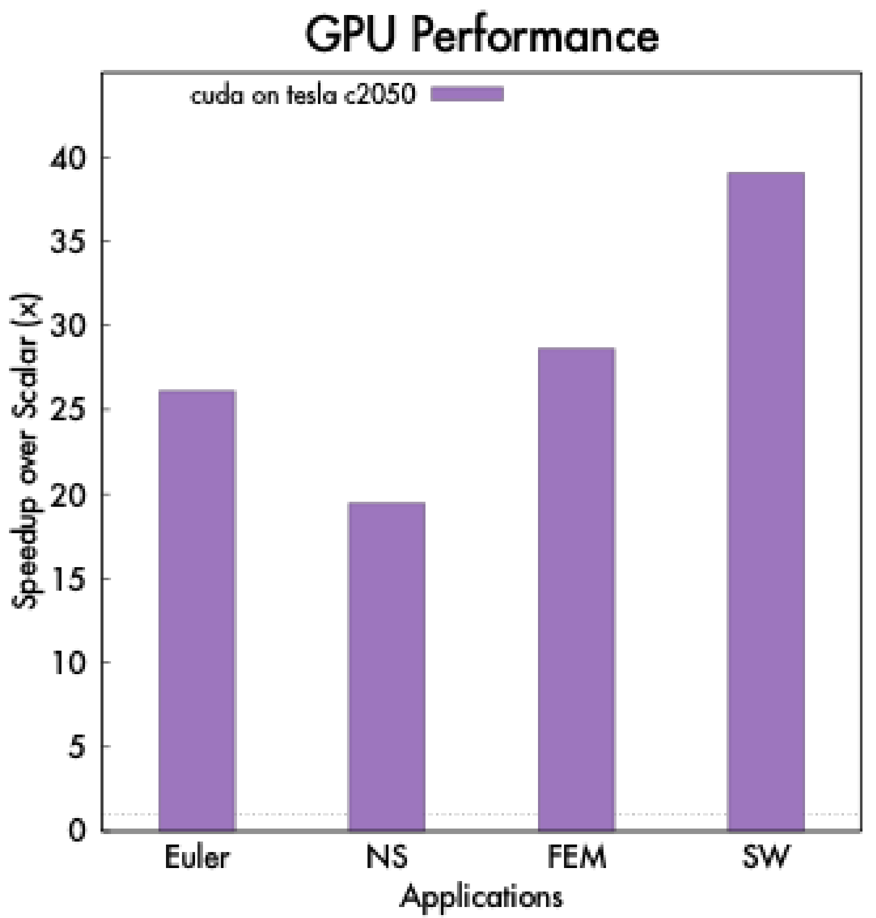
4-socket 6-core 2.66Ghz Xeon CPU per node (24 cores), 16GB RAM per node. 256 nodes, 8 cores per node



GPU Performance

Tesla C2050, Double Precision, compared to

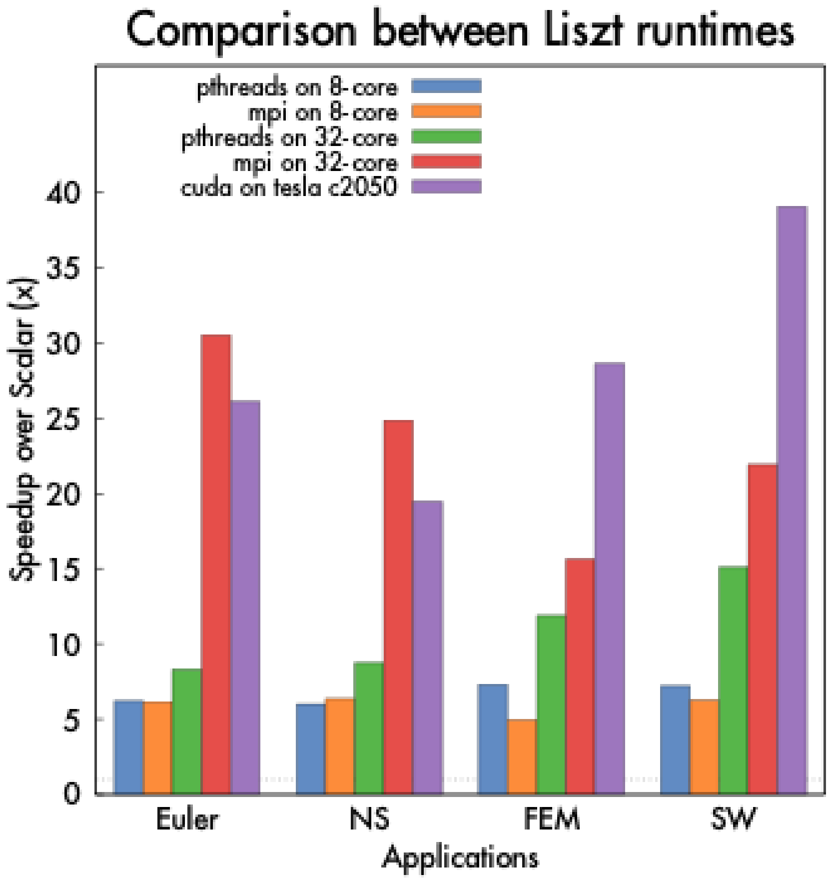
single core, Nehalem E5520 2.26Ghz, 8GB RAM



Portability

Tested both pthreads (coloring) and MPI (partitioning) runtime on:

- 8-core Nehalem E5520 2.26Ghz, 8GB RAM
- 32-core Nehalem-EX X7560 2.26GHz, 128GB RAM



Takeaways

- Bottom-up (from applications) approach worked for us
  - First attempted to build this as a library
  - Then invented stencil detection to automate targetting API
- Examples are key
  - Most of the back-end was “extracted” from exampe codes
- Static-Dynamic program analysis split is annoying
  - Makes code obtuse – lots of generated code for analysis
  - Makes some things very hard (adaptive meshes…)
  - Make the compiler part of the runtime?(ArBB…?)
- Shared-access machines makes me want to shoot myself in the face