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

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Motivation

Physics is complex & changing

Software must handle complexity & changing nature of:
  - physics models,
  - algorithms,
  - hardware

Hardware is complex & changing
  - multicore/manycore
  - hybrid CPU/GPU or other accelerators

Software

Physics Models

Algorithms & Solvers

Monday, February 20, 12
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
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.
Register all expressions.

- Each “expression” calculates one or more field quantities, and this is indicated to the registry.
- Each expression advertises its direct dependencies

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

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\Gamma = \Gamma(T, p, y_i)
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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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\[ \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{u}) \]
\[ \frac{\partial \rho \vec{u}}{\partial t} = -\nabla \cdot (\rho \vec{u} \vec{u}) - \nabla \cdot \tau - \nabla p + \rho \vec{g} \]
\[ \frac{\partial \rho e_0}{\partial t} = -\nabla \cdot (\rho e_0 \vec{u}) - \nabla \cdot (\rho \vec{u}) - \nabla \cdot (\tau \vec{u}) - \nabla \cdot q \]
\[ \frac{\partial \rho y_i}{\partial t} = -\nabla \cdot (\rho y_i \vec{u}) - \nabla \cdot \vec{J}_i + s_i \]
**Example: multiphase flows**

- Do we need logic in formulating each transport equation to indicate if “multiphase” is turned on?

\[
\begin{align*}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho \vec{u}) + s_\rho \\
\frac{\partial \rho \vec{u}}{\partial t} &= -\nabla \cdot (\rho \vec{u} \vec{u}) - \nabla \cdot \tau - \nabla \cdot p + \rho \vec{g} + s_{\rho \vec{u}} \\
\frac{\partial \rho e_0}{\partial t} &= -\nabla \cdot (\rho e_0 \vec{u}) - \nabla \cdot (\rho \vec{u}) - \nabla \cdot (\tau \vec{u}) - \nabla \cdot q + s_{\rho e_0} \\
\frac{\partial \rho y_i}{\partial t} &= -\nabla \cdot (\rho y_i \vec{u}) - \nabla \cdot \vec{J}_i + s_i + s_{\rho y_i}
\end{align*}
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\end{align*}
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Example: multiphase flows

- Do we need logic in formulating each transport equation to indicate if “multiphase” is turned on?

“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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Additional Model Complexity

Example: multiphase flows

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\frac{\partial \rho e_0}{\partial t} = -\nabla \cdot (\rho e_0 \vec{u}) - \nabla \cdot (p \vec{u}) - \nabla \cdot (\tau \vec{u}) - \nabla \cdot \vec{q} + s_{\rho e_0}
\]

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\frac{\partial \rho y_i}{\partial t} = -\nabla \cdot (\rho y_i \vec{u}) - \nabla \cdot \vec{J}_i + s_i + s_{\rho y_i}
\]

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

\( \frac{\partial Q}{\partial t} \) doesn’t directly advertise a dependency on \( s_Q \).
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!
“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.
“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.

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Serialization point - push resources into data parallel on E.
“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)

Prioritize D (may push resources into “D” if possible)
“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.
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• resources may be dynamically migrated between thread pool associated with task graph to threads associated with data-parallel execution (within a node)

Serialization point - push resources into data parallel on C.
“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)

Serialization point - push resources into data parallel on A.
Graph analysis indicates theoretical parallelizability and speedup.

<table>
<thead>
<tr>
<th>n</th>
<th>P</th>
<th>S_∞</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0.89</td>
<td>7.5</td>
</tr>
<tr>
<td>16</td>
<td>0.94</td>
<td>13.7</td>
</tr>
<tr>
<td>32</td>
<td>0.97</td>
<td>28.6</td>
</tr>
</tbody>
</table>

- 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!

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

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

Loop Fusing

1 loop, \( \lambda \) and \( \partial \phi / \partial x_i \) held as temporaries on inner loops.
Domain-Specific Languages

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

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

\[
\text{rhs} \Leftarrow Dx( Rx(\Gamma) \ast Gx(\phi) ) + Dy( Ry(\Gamma) \ast Gy(\phi) ) + Dz( Rz(\Gamma) \ast Gz(\phi) ) + Sphi
\]

DSL hides details of implementation - fast refactors

Monday, February 20, 12
Memory Management - Pool Allocation

Stage 1

'I', 'A' allocated statically

Static fields
I A

Dynamic fields

Direction of Execution

A
B
C
D
E
F
G
H
I

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Memory Management - Pool Allocation

Stage 1
- ‘I’, ‘A’ allocated statically

Stage 2
- ‘F’, ‘G’, ‘H’ allocated

Static fields: I, A
Dynamic fields: F, G, H
Memory Management - Pool Allocation

- **Stage 1**: ‘I’, ‘A’ allocated statically
- **Stage 2**: ‘F’, ‘G’, ‘H’ allocated
- **Stage 3**: ‘E’ allocated

**Static fields**: I, A

**Dynamic fields**: F, G, H, E

Direction of Execution
Memory Management - Pool Allocation

Static fields:
- I
- A

Dynamic fields:
- B
- D
- E

Stage 1:
- ‘I’, ‘A’ allocated statically

Stage 2:
- ‘F’, ‘G’, ‘H’ allocated

Stage 3:
- ‘E’ allocated

Stage 4:
- ‘B’, ‘D’ allocated

Direction of Execution
Memory Management - Pool Allocation

Stage 1:
- ‘I’, ‘A’ allocated statically

Stage 2:
- ‘F’, ‘G’, ‘H’ allocated
- ‘I’, ‘A’ allocated

Stage 3:
- ‘E’ allocated

Stage 4:
- ‘B’, ‘D’ allocated

Stage 5:
- ‘E’ released
- ‘C’ allocated

Static fields:
- I, A

Dynamic fields:
- B, D, C
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

- Task Scheduler
  - Is task GPU-ready?
    - yes: Execute on CPU
    - no: Does execution time exceed data movement time?
      - yes: Execute on GPU
      - no: Execute on CPU

- DSL provides support for GPU deployment of operations.
Current Work - Hybrid CPU/GPU

- 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.

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

Task Scheduler

- Is task GPU-ready?
- Does execution time exceed data movement time?
- Execute on CPU
- Execute on GPU
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.