Software Abstractions for Extreme-Scale Scalability of Computational Frameworks

Martin Berzins

1. Background, motivation, Directed Acyclic Graph software
2. A DAG Example the Uintah Software
3. Engineering for Scalability with DAGs
4. Conclusions

DAG Software Hype?
Here?
Or here?

Here?

DOE ASCI (97-10), NSF, DOE NETL+NNSA ARL
NSF, INCITE, XSEDE
BACKGROUND
MOTIVATION DAGs, SOFTWARE
Extreme Scale Research and teams in Utah

**Energetic Materials:** Chuck Wight, Jacqueline Beckvermit, Joseph Peterson, Todd Harman, Qingyu Meng NSF PetaApps 2009-2014 $1M, P.I. MB

**PSAAP Clean Coal Boilers:** Phil Smith (P.I.), Jeremy Thornock James Sutherland etc Alan Humphrey John Schmidt DOE NNSA 2013-2018 $16M (MB Cs lead)

**Electronic Materials by Design:** MB (PI) Dmitry Bedrov, Mike Kirby, Justin Hooper, Alan Humphrey Chris Gritton, + ARL TEAM 2011-2016 $12M

**Software team:** Qingyu Meng*, John Schmidt, Alan Humphrey, Justin Luitjens**, James Sutherland

* Now at Google

** Now at NVIDIA
The Exascale challenge for Future Software?

Harrod SC12: “today’s bulk synchronous (BSP), distributed memory, execution model is approaching an efficiency, scalability, and power wall.”

Sarkar et al. “Exascale programming will require prioritization of critical-path and non-critical path tasks, adaptive directed acyclic graph scheduling of critical-path tasks, and adaptive rebalancing of all tasks……”

“DAG Task-based programming has always been a bad idea. It was a bad idea when it was introduced and it is a bad idea now “ Parallel Processing Award Winner

Much architectural uncertainty, many storage and power issues. Adaptive portable software needed

Power needs force use of accelerators
Some Historical Background

  - Graphical rep. for parallel programs
  - Cost model
  - Compile time cost assignment
  - Macro-data flow for execution
  - Compile time schedule
  - Prototype implementation 20 processors
- Charm++  Sanjay Kale et al. 1990s onward
- Uintah  Steve Parker 1998 onward

Present Day

Much work on task graphs –
e.g. O. Sinnen “Task Scheduling for Parallel Systems”
Task Graph Based Languages/Frameworks

Uintah Taskgraph based PDE Solver (Parker 1998)

Plasma (Dongarra): DAG based Parallel linear algebra software

StarPU Task Graph Runtime

Kale (1990) Charm++: Object-based Virtualization
Why does Dynamic Execution of Directed Acyclic Graphs Work Well?

- Eliminate spurious synchronizations points
- Have multiple task-graphs per multicore (+ gpu) node – provides excess parallelism - slackness
- Overlap communication with computation by executing tasks as they become available – avoid waiting (use out-of-order execution).
- Load balance complex workloads by having a sufficiently rich mix of tasks per multicore node that load balancing is done per node.
Some components have not changed as we have gone from 600 to 600K cores

- **Application Specification** via ICE MPM ARCHES or NEBO/WASATCH DSL

- **Abstract task-graph** program that

- Is compiled for

- Executes on: **Runtime System** with: asynchronous out-of-order execution, work stealing, Overlap communication & computation. Tasks running on cores and accelerators

- **Scalable I/O** via Visus PIDX

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**Uintah(X) Architecture Decomposition**
**Uintah Patch, Variables and AMR Outline**

ICE is a cell-centered finite volume method for Navier Stokes equations.

**ICE Structured Grid Variable (for Flows)** are Cell Centered Nodes, Face Centered Nodes.

**Unstructured Points (for Solids)** are MPM Particles.

**ARCHES** is a combustion code using several different radiation models and linear solvers.

**Uintah:MD** based on Lucretius is a new molecular dynamics component.

- **Structured Grid + Unstructured Points**
- **Patch-based Domain Decomposition**
- **Regular Local Adaptive Mesh Refinement**
- **Dynamic Load Balancing**
  - Profiling + Forecasting Model
  - Parallel Space Filling Curves
- **Works on MPI and/or thread level**
void Burger::scheduleTimeAdvance(const LevelP& level, SchedulerP& sched)
{
    ....
    task->requires(Task::OldDW, u_label, Ghost::AroundNodes, 1);
    task->requires(Task::OldDW, sharedState_->get_delt_label());
    task->computes(u_label);
    sched->addTask(task, level->eachPatch(), sharedState_->allMaterials());
}

25 cubed patches
8 patches
One level of halos

Get old solution from old data warehouse
One level of halos
Compute new solution
Burgers Equation code

\[ \frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x} = 0 \]

```cpp
void Burger::timeAdvance(const ProcessorGroup*, const PatchSubset* patches,
const MaterialSubset* matls, DataWarehouse* old_dw, DataWarehouse* new_dw)
//Loop for all patches on this processor
{ for(int p=0;p<patches->size();p++){
//Get data from data warehouse including 1 layer of "ghost" nodes from surrounding patches
  old_dw->get(u, lb_->u, matl, patch, Ghost::AroundNodes, 1);

// dt, dx Time and space increments
  Vector dx = patch->getLevel()->dCell();
    old_dw->get(dt, sharedState_->get_delt_label());

// allocate memory for results new_u
  new_dw->allocateAndPut(new_u, lb_->u, matl, patch);

// define iterator range l and h ...... lots missing here and Iterate through all the nodes
  for(NodeIterator iter(l, h);!iter.done(); iter++){
        IntVector n = *iter;
        double dudx = (u[n+IntVector(1,0,0)] - u[n-IntVector(1,0,0)]) /(2.0 * dx.x());
        double du = - u[n] * dt * (dudx);
        new_u[n]= u[n] + du;
  }
}
```
Uintah Directed Acyclic (Task) Graph-Based Computational Framework

Each task defines its computation with required inputs and outputs

Uintah uses this information to create a task graph of computation (nodes) + communication (along edges)

Tasks do not explicitly define communications but only what inputs they need from a data warehouse and which tasks need to execute before each other.

Communication is overlapped with computation

Task graph is executed adaptively and sometimes out of order, inputs to tasks are saved

Tasks get data from OLD Data Warehouse and put results into NEW Data Warehouse
Runtime System
The nodal task soup

Task Graph Structure on a Multicore Node with multiple patches

This is not a single graph. Multiscale and Multi-Physics merely add flavor to the “soup”.
The DAG Approach is not a silver bullet

**Uintah Phase 1 1998-2005** – overlap communications with computation. Static task graph execution standard data structures one MPI process per core. No AMR.

**Uintah Phase 2 2005-2010** improved fast data structures, load balancer. AMR to 12k cores, then 100K cores using new approach before data structures cause problems. Out of order and dynamic task execution.

**Uintah Phase 3 2010-** Hybrid model. Theaded runtime system on node. One MPI process and one data warehouse per node. Multiple cores and GPUs grab tasks as needed. Fast scalable use of hypre for linear equations.
UINTAH SCALABILITY
Explosives Problem 1 Fluid-Structure Benchmark
Example: AMR MPMICE

A PBX explosive flow quickly pushing a piece of its metal container

Grid Variables: Fixed number per patch, relative easy to balance
Particle Variables: Variable number per patch, hard to load balance
Thread/MPI Scheduler (De-centralized)

- One MPI Process per Multicore node
- All threads directly pull tasks from task queues execute tasks and process MPI sends/receives
- Tasks for one patch may run on different cores
- One data warehouse and task queue per multicore node
- Lock-free data warehouse enables all cores to access memory quickly
Uintah Runtime System

Task Graph

Internal Task Queue
Comm Records
External Task Queue

Execution Layer (runs on multiple cores)

Select Task & Post MPI Receives
Check Records & Find Ready Tasks
Select Task & Execute Task
Post Task MPI Sends

Data Management

Data Warehouse (one per-node)

Network

Shared Objects (one per node)
New Hybrid Model Memory Savings: Ghost Cells

MPI:

Raw Data: 49152 doubles
MPI buffer: 28416 doubles
Total: 75K doubles

Thread/MPI:

31360 doubles
10624 doubles
40K doubles

(example on Kraken, 12 cores/node, 98K core 11% of memory needed)
Task prioritization algorithms

Executing the task pool in different ways leads to different communications patterns.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Random</th>
<th>FCFS</th>
<th>PatchOrder</th>
<th>MostMsg.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Queue Length</td>
<td>3.11</td>
<td>3.16</td>
<td>4.05</td>
<td>4.29</td>
</tr>
<tr>
<td>Wait Time</td>
<td>18.9</td>
<td>18.0</td>
<td>7.0</td>
<td>2.6</td>
</tr>
<tr>
<td>Overall Time</td>
<td>315.35</td>
<td>308.73</td>
<td>187.19</td>
<td>139.39</td>
</tr>
</tbody>
</table>

Prioritize tasks with external communications over purely internal ones.
Granularity Effect

- Decrease patch size
  - (+) Increase queue length
  - (+) More overlap, lower task wait time
  - (+) More patches, better load balance
  - (-) More MPI messages
  - (-) More regrid overheads

- Other Factors
  - Problem size
  - Implied task level parallelism
  - Interconnection bandwidth and legacy
  - CPU cache size

- Solution- Self Tuning?

![Graph showing ICE Wait Time and Task Ready Queue Length](image1.png)

![Graph showing ICE with different patch sizes (Kraken, with 24K cores)](image2.png)
Nodal Performance and Global Scalability on Titan

Scaling fine on Jaguar XK6
Breakdown on Jaguar XK7 with more faster cores and a faster network – needed a rewrite of Data Warehouse to allow cores faster access

One flow with particles moving
3-level AMR MPM ICE 70% efficiency
At 256K cores vs 16K cores
Lock-Free Data Structures

Global scalability depends on the details of nodal run-time system. Change from Jaguar to Titan – more faster cores and faster communications broke our Runtime System which worked fine with locks previously.

- Using atomic instruction set
- Variable reference counting
  - `fetch_and_add`, `fetch_and_sub`, `compare_and_swap`
  - both read and write simultaneously
- Data warehouse
  - Redesigned variable container
  - Update: `compare_and_swap`
  - Reduce: `test_and_set`
Scalability is at least partially achieved by not executing tasks in order e.g. AMR fluid-structure interaction.

Straight line represents given order of tasks. Green X shows when a task is actually executed. Above the line means late execution while below the line means early execution took place. More “late” tasks than “early” ones as e.g.

TASKS: 1 2 3 4 5

Early | Late execution

1 4 2 3 5
Weak Scaling AMR+MPM ICE
M = Mira, T=Titan, S=Stampede

Only 2 patches per core
Includes packing, unpacking, and data warehouse

Only 8 interior patches from 32
Deflagration wave moves at ~400m/s not all explosive consumed. Detonation wave moves 8500m/s all explosive consumed.

NSF funded modeling of Spanish Fork Accident 8/10/05

Speeding truck with 8000 explosive boosters each with 2.5-5.5 lbs of explosive overturned and caught fire

Experimental evidence for a transition from deflagration to detonation?
At every stage when we move to the next generation of problems, some of the algorithms and data structures need to be replaced.

Scalability at one level is no certain indicator for problems or machines. An order of magnitude larger...
Complex fluid-structure interaction problem with adaptive mesh refinement, see SC13/14 paper NSF funding.
Summary of Scalability Improvements

(i) Move to a one MPI process per multicore node reduces memory to less than 10% of previous for 100K+ cores

(ii) Use optimal size patches to balance overhead and granularity 16x16x16 to 30x30x30.

(iii) Use only one data warehouse but allow all cores fast access to it, through the use of atomic operations.

(iv) Prioritize tasks with the most external communications

(v) Use out-of-order execution when possible
An Exascale Design Problem - Alstom Clean Coal Boilers

For 350MWe boiler problem. LES resolution needed: 1mm per side for each computational volume = $9 \times 10^{12}$ cells. This is one thousand times larger than the largest problems we solve today.

Prof. Phil Smith Dr Jeremy Thornock ICSE
Existing Simulations of Boilers using ARCHES in Uintah

(i) Traditional Lagrangian/RANS approaches do not address well particle effects
(ii) LES has potential to predict oxy-coal flames and to be an important design tool
(iii) LES is “like DNS” for coal, but 1mm mesh needed to capture phenomena

Structured, finite-volume method, Mass, momentum, energy with radiation
Higher-order temporal/spatial numerics, LES closure, Tabulated chemistry
PDF mixing models, DQMOM, modeling particles
Uncertainty Quantified
Runs on a Small Prototype Boiler

Red is experiment
Blue is simulation
Green is consistent

Absence of scales for commercial reasons

[Source: Jeremy Thornock]
Linear Solves arises from Low Mach Number Navier –Stokes Equations

\[ \nabla^2 p = R, \text{ where } R = \nabla F + \frac{\partial^2 p}{\partial t^2} \]

Use Hypre Solver from LLNL
Preconditioned Conjugate Gradients on regular mesh patches used
Multi-grid pre-conditioner used
Careful adaptive strategies needed to get scalability

Each Mira Run is scaled wrt the Titan Run at 256 cores
Note these times are not the same for different patch sizes.

Weak Scalability of Hypre Code
Express complex pde functions as DAG - automatically construct algorithms from expressions

Define field operations needed to execute tasks (fine grained vector parallelism on the mesh)

User writes only field operations code. Supports field & stencil operations directly - no more loops!

Strongly typed fields ensure valid operations at compile time. Allows a variety of implementations to be tried without modifying application code.

Scalability on a node - use Uintah infrastructure to get scalability across whole system.

**NEBO/Wasatch Example**

**Energy equation**

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) + \nabla \cdot J_h + \text{terms} = 0
\]

Enthalpy diffusive flux

\[
J_h = -\lambda(T,Y_j)\nabla T - \sum_{i=1}^{n} h_i J_i
\]

\[
J_i = -\sum_{j=1}^{ns} D_{ij}(T,Y_j)\nabla Y_j - D_{ij}^T(T,Y_j)\nabla T
\]

[Sutherland Earl Might]
- Use **CUDA Asynchronous API**
- **Automatically** generate CUDA streams for task dependencies
- **Concurrently** execute kernels and memory copies
- **Preload** data before task kernel executes
- **Multi-GPU** support
Wasatch – Nebo Recent Milestones

- Wasatch is solving (nonreacting miniboiler) ~3-4x speedup over the non-DSL approach.
- New Nebo backend for CPU resulted in 20-30% speedup in the entire Wasatch code base.
- Much of the Wasatch code base is GPU-ready.
- Arches plus SpatialOps & Nebo EDSL being scoped.

Good GPU scaling with (>32^3 per patch).
Loop fusion (heavy GPU kernels) needed e.g. “coupled source & diffusion”
DESIGNING FOR EXASCALE

Clear trend towards accelerators e.g. GPU but also Intel MIC – new NSF “Stampede” 10-. 15PF Balance factor = flops/bandwidth - high

GPU performance “ok” for stencil-based codes ,2x over multicore cpu estimated and achieved for ICE . Similar results by others. Network and memory performance more slowly growing than cpu/gpu performance. GPU perf.of ray-tracing radiation method is 100x cpu

Overlapping and hiding Communications essential

![Graph of RMCRT and MPMICE performance](image)
NVIDIA AMGX Linear Solvers on GPUs

- Fast, scalable iterative gpu linear solvers for packages e.g.,
- Flexible toolkit provides GPU accelerated Ax = b solver
- Simple API for multiple apps domains.
- Multiple GPUs (maybe thousands) with scaling

Key Features
- Ruge-Steuben algebraic MG
- Krylov methods: CG, GMRES, BiCGStab,
- Smoothers and Solvers: Block- Jacobi, Gauss-Seidel, incomplete LU,
- Flexible composition system
- MPI support OpenMP support, Flexible and high level C API,

Free for non-commercial use
Utah access via Utah CUDA COE.
DESIGNING FOR EXASCALE

Clear trend towards accelerators e.g. GPU but also Intel MIC – NSF “Stampede” Balance factor = flops/bandwidth – high. PORTABILITY IS THE KEY ISSUE: NEW CODE - use Wasatch to generate code for GPUs and MICs. How do we handle the challenge of existing code?

Kokkos: A Layered Collection of Libraries

- Standard C++, Not a language extension
  - In spirit of TBB, Thrust & CUSP, C++AMP, LLNL’s RAJA, ...
  - Not a language extension like OpenMP, OpenACC, OpenCL, CUDA, ...
- Uses C++ template meta-programming
- Multidimensional Arrays, with a twist
  - Layout mapping: multi-index (i,j,k,...) ↔ memory location
    - Choose layout to satisfy device-specific memory access pattern
  - Layout changes are invisible to the user code

[source Carter Edwards and Dan Sunderland]
Evaluate Performance Impact of Array Layout
[Edwards and Sunderland]

- Molecular dynamics computational kernel in miniMD
- Simple Lennard Jones force model:
  \[ F_i = \sum_{j, r_{ij} < r_{cut}} 6\varepsilon \left( \frac{\varsigma}{r_{ij}} \right)^7 - 2 \left( \frac{\varsigma}{r_{ij}} \right)^{13} \]
- Atom neighbor list to avoid N\(^2\) computations

```c
pos_i = pos(i);
for( jj = 0; jj < num_neighbors(i); jj++) {
    j = neighbors(i,jj);
    r_ij = pos_i - pos(j); //random read 3 floats for pos
    if (|r_ij| < r_cut) f_i += 6*\varepsilon*((s/r_ij)^7 - 2*(s/r_ij)^13)
}
f(i) = f_i;
```

- Test Problem
  - 864k atoms, \(~77\) neighbors
  - 2D neighbor array
  - Different layouts CPU vs GPU
  - Random read ‘pos’ through GPU texture cache

- Large performance loss with wrong array layout
Proposed Uintah(X) Architecture Decomposition

Applications code

Abstract C++ Task Graph Form

Compilation into C++ Cuda etc

Adaptive Execution of tasks

On specific processors

Proposed Uintah(X) Architecture Decomposition
Resilience

- Need interfaces at system level to help us consider:
  - Core failure – reroute tasks
  - Comms failure – reroute message
  - Node failure – need to replicate patches use an AMR type approach in which a coarse patch is on another node. In 3D has 12.5% overhead – suggested by Qingyu Meng Mike Heroux and others.

- Will explore this from fall 2014 onwards. Just how bad is the problem?
Summary

• DAG abstraction important for achieving scaling
• Layered approach very important for not needing to change applications code
• Scalability still requires much engineering of the runtime system.
• General approach very powerful indeed.
• Obvious applicability to new architectures
• DSL approach very important very future
• Scalability still a challenge even with DAG approach – which does work amazingly well, e.g. for fluid-structure calculations
• GPU and MIC development ongoing
• The approach used here shows promise for very large core and GPU counts but using these architectures is an exciting challenge
ARL: Multi-scale Modeling of Electronic Materials
Utah, Boston, RPI, Chicago, Harvard, Brown, Penn State

Vision: Longer lasting batteries and fuel Cells for extreme environments
New generation of LEDs and night-vision
New materials

• Complex problems require differing scales
  Example: Battery Cathode (Atomistic/CG + MPM)
  Mesoscopic (or larger) cathode particle mechanical response via MPM. Microscopic particle/electrolyte interactions at Atomistic/CG scale

Computational Challenges
(i) Marrying simulation techniques across multiple orders of magnitudes.
(ii) Quantifying Uncertainty across multiple scales
Weak and Strong Scalability:
Problem size $n$ on $p$ cores takes time $T(n,p)$

**Strong Scalability**

$$T(n, p) = \frac{T(n, 1)}{p}$$

Try to solve the same problem $p$ times more quickly on $p$ cores

**Weak Scalability**

$$T(np, p) = T(n, 1)$$

Solve a problem that is $p$ times as large in the same time on $p$ cores

**Theorem**

Both weak and strong scalability only if linear complexity

[Tirado + Martin] 1998

$$T(n, 1) = \alpha n$$
Today’s machines used in this talk

<table>
<thead>
<tr>
<th>SYSTEM</th>
<th>Vendor/ Type</th>
<th>CPUs and Accelerators</th>
<th>Cores</th>
<th>Mem/ Node</th>
<th>Inter-conn.</th>
<th>Peak Pflop</th>
</tr>
</thead>
<tbody>
<tr>
<td>TITAN</td>
<td>Cray XK7</td>
<td>AMD Opteron 2.6Ghz</td>
<td>299008 18K x 2496</td>
<td>32GB</td>
<td>Cray Gemini</td>
<td>27</td>
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<td></td>
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<td>NVIDIA KEPLER</td>
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<tr>
<td>Stampede</td>
<td>Dell Zeus</td>
<td>Intel Sandybridge 2.7GHz</td>
<td>102400 390400</td>
<td>32GB</td>
<td>Infiniband</td>
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<td>Intel Xeon Phi</td>
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<tr>
<td>Mira</td>
<td>IBM Blue Gene Q</td>
<td>Power PC A2 1.6Ghz</td>
<td>786432</td>
<td>16GB</td>
<td>5D Torus</td>
<td>10</td>
</tr>
</tbody>
</table>

NSFs Kraken and DOE's Titan, DoD machines and local HP machines are our workhorses.

THESE MACHINES WILL SEEM “SMALL” IN 2025 and will the equivalent of large regional or lab machines but are ranked 2, 7 and 4 in the world today
GPU Task Management

With Uintah’s knowledge of the task-graph, task data can be automatically transferred asynchronously to the device before a GPU task executes.

- All device memory allocations and asynchronous transfers handled automatically.
- Can handle multiple devices on-node.
- All device data is made available to component code via convenient interface.

1. Pin this memory with `cudaHostRegister()`
2. `cudaMemcpyAsync(H2D)`
3. Result back on host
4. `cudaMemcpyAsync(D2H)`
5. Component requests D2H copy here
6. Free pinned host memory

Call-back executed here (kernel run)
Memory Savings

- Global Meta-data copies
  - 60 bytes or 7.5 doubles per patch
  - Each copy per core vs Each copy per node
- MPI library buffer overhead
- Results:

\[ \text{Ratio} = \frac{\text{Thread MPI memory usage}}{\text{MPI memory usage}} \times 100\% \]

<table>
<thead>
<tr>
<th>Cores</th>
<th>3072</th>
<th>6144</th>
<th>12288</th>
<th>24576</th>
<th>49152</th>
<th>98304</th>
</tr>
</thead>
<tbody>
<tr>
<td>Percent</td>
<td>61%</td>
<td>47%</td>
<td>36%</td>
<td>27%</td>
<td>18%</td>
<td>11%</td>
</tr>
</tbody>
</table>

AMRICE: Simulation of the transport of two fluids with a prescribed initial velocity of Mach two: 435 million cells, strong scaling runs on Kraken
Uintah Applications

Explosions

Angiogenesis

Industrial Flares

Micropin Flow

Sandstone Compaction

Foam Compaction

Carbon capture and cleanup

Shaped Charges