Foundations of Data-Parallel Particle Advection

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Scientific Data Analysis and Specifically Particle Tracing

**General**

- Big science => HPC analysis
- Data analysis => data movement
- Parallel => distributed memory data parallel
- Most analysis algorithms are not up to the challenge
  - Either serial or shared memory parallel
  - Communication and I/O are scalability killers

**Particle Tracing**

- Data sizes are large, and large numbers of particles are needed (hundreds of thousands) for accurate further analysis of field line features.
- High communication volume and data-dependent load balance make particle tracing challenging to parallelize and scale efficiently.
Moving from Postprocessing to Run-Time Scientific Data Analysis in HPC

Postprocessing particle tracing and visualization

Run-time particle tracing and postprocessing visualization
The Need for Parallel Particle Tracing

When data sizes are too large to move or process serially, parallel particle tracing needs to be executed on HPC machines. Results are available sooner, access to all data at full resolution is possible.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Grid size</th>
<th>Data size (GB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAX</td>
<td>$2048^3$</td>
<td>98</td>
</tr>
<tr>
<td>RTI</td>
<td>$2304 \times 4096 \times 4096$</td>
<td>432</td>
</tr>
<tr>
<td>Flame</td>
<td>$1408 \times 1080 \times 1100$ x 32 time steps</td>
<td>608</td>
</tr>
</tbody>
</table>

Test Data Sizes

Image courtesy Mark Petersen, Daniel Livescu, LANL. Code: CFDNS

Image courtesy Ray Grout, NREL, Hongfeng Yu, Jackie Chen, SNL Code: S3D

Rayleigh-Taylor Instability

MAX Experiment

Flame Stabilization

Image courtesy Paul Fischer, Aleks Obabko, ANL. Code: Nek5000
1. Group data into blocks and assign blocks to processors.

2. Each voxel contains a velocity vector.

3. Advect particles along velocity vectors.

4. Exchange particles among processes when they reach the block boundary.

5. Repeat 3, 4.

$8^3 = 512$ voxels
64 blocks
3 Processes
OSUFlow and DIY

OSUFlow is a library of serial / parallel particle tracing functions that is parallelized using a library called DIY that helps the user write data-parallel analysis algorithms by decomposing a problem into blocks and communicating items between blocks.

**OSUFlow Features**
- Static / time-varying flows
- Regular / rectilinear / curvilinear / unstructured grids
- Fixed / adaptive step sizes
- Various integration methods

**DIY Features**
- Parallel I/O to/from storage
- Domain decomposition
- Network communication
- Utilities

![DIY Usage and Library Organization Diagram]
Nine Things That DIY Does

1. Separate analysis ops from data ops
2. Group data items into blocks
3. Assign blocks to processes
4. Group blocks into neighborhoods
5. Support multiple instances of 2, 3, and 4
6. Handle time
7. Communicate between blocks in various ways
8. Read data and write results
9. Integrate with other libraries and tools
• Neighborhoods provide limited-range communication among arbitrary groupings of blocks with distributed, scalable data structures
• DIY provides different options within a neighborhood including sending an item to all neighbors near enough to receive it and periodic boundary conditions. Items are enqueued are subsequently exchanged (2 steps). Items are user-defined.

Two examples of 3 out of a total of 25 neighborhoods
It’s About Time

- Time often goes forward only
- Usually do not need all time steps at once

<table>
<thead>
<tr>
<th>4D</th>
<th>3D</th>
<th>1D</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Xmax, Ymax, Zmax, Tmax)</td>
<td>(Xmax, Ymax, Zmax)</td>
<td>( Tmin)</td>
</tr>
<tr>
<td>(Xmin, Ymin, Zmin, Tmin)</td>
<td>(Xmin, Ymin, Zmin)</td>
<td>( Tmax)</td>
</tr>
</tbody>
</table>

4D Block

3D Spatial Extent

1D Temporal Extent

Hybrid 3D/4D time-space decomposition. Time-space is represented by 4D blocks that can also be decomposed such that time blocking is handled separately.
Configurable 3D / 4D Hybrid Algorithm

Internally, all blocks are 4D, but we allow separate grouping in space (blocks) and time (epochs) to control how much data are kept in-core in each epoch. This enables time-varying data to be traced natively in 4D, without requiring the entire 4D dataset to be resident in memory.

Algorithm

- decompose domain into blocks
- assign blocks to processes

for (epochs) {
   read my process’ data blocks
   for (rounds) {
      for (my blocks) {
         advect particles
      }
      exchange particles
   }
}

Data structure
Adjustable Synchronization Communication Algorithm

for (blocks in my neighborhood) {
    pack and send messages of block IDs and particle counts
    pack and send messages of particles
}

wait for enough IDs and counts to arrive
for (IDs and counts that arrived) {
    receive particles
}
Nonblocking point-to-point and waiting for all messages to arrive (wait factor = 1.0) offers little improvement over all-to-all communication, but dialing down the wait factor helps significantly.

MAX experiment data. Point to point with wait factor = 1.0 is virtually the same as all to all.

Flame stabilization data. Less synchronization (wait factor = 0.1) improves performance.
Particle tracing of ¼ million particles in a $2048^3$ thermal hydraulics dataset results in strong scaling to 32K processes and an overall improvement of $2X$ over earlier algorithms. Most of this improvement comes from the wait factor. The left plot includes end-to-end time, including I/O, computation, and communication. The right image shows 8 thousand particles, much fewer than were actually tested.
The Problem of Load Balancing

Computational load is data dependent: data blocks containing vortices (sinks) attract particles and have high angular frequency requiring thousands more advection steps to compute than blocks with homogeneous flow. In the following slides, we evaluate three solutions: particle termination, multiblock assignment, and dynamic block re-assignment.

One process containing 4 blocks, with one block containing a vortex, can affect the load balance of the entire program execution.
Particle Termination

**Problem:** A busy process causes others to wait, which propagates throughout the system.

**Solution:** Particles that don’t exit the current block after one round are terminated. There is no loss of information because these particles have near-zero velocity.

Jumpshots of 128 processes: process 105 is computation-bound and causes all others to wait. Terminating particles that do not leave the current block reduces maximum computation time and overall time.
Multiblock Assignment

Decomposing the domain into a larger number of smaller blocks helps, to a limit. Computational hot-spots are more likely to be amortized over a greater number of processes. Limiting factor: smaller blocks incur less computation and more communication because surface area / volume increases.

Example of 512 voxels decomposed into 64 blocks and assigned to 3 processes. Each process contains 21 or 22 blocks.

Decompositions of 1, 2, 4, 8, and 16 blocks per process in the MAX dataset, 512^3, 8K particles. Higher block numbers reduce the overall execution time. Early particle termination not applied in these tests.
MAX Experiment Results

Strong scaling, $512^3$, $1024^3$, $2048^3$ data, 128K particles, 1 time-step

Strong Scaling For Various Data Sizes

Data courtesy Aleks Obabko and Paul Fischer, ANL

Platform: IBM Blue Gene/P
Rayleigh-Taylor Results

Weak scaling, 2304 x 4096 x 4096 data, 16K to 128K particles, 1 time-step

Data courtesy Mark Petersen and Daniel Livescu, LANL

Platform: IBM Blue Gene/P
Flame Stabilization Results

Weak scaling, 1408 x 1080 x 1100 data, 512 to 16K particles, 1 to 32 time-steps

Data courtesy Ray Grout, NREL and Jackie Chen, SNL

Platform: IBM Blue Gene/P
VTK Integration

VTK Parallel Reader → Adapter → OSUFlow → Adapter → VTK Renderer

Top: Streamlines of thermal hydraulics. Bottom: Pathlines of tornado

Top: Mesh for office airflow. Bottom: streamlines for office airflow

Top: Mesh for blunt fin. Bottom: streamlines for blunt fin

Courtesy Zhanping Liu and Jimmy Chen
Summary

**Keys to Successes**

- Configurable time-space data structure with variable size epochs and blocks
  - Load as many time steps into memory as possible
- Communication algorithm with adjustable synchronization
  - Less synchronization is better, eg., wait for 10% of pending messages
- Simple load balancing strategies
  - Multiple blocks per process, particle termination

**Ongoing / future work**

- Continuing to study dynamic load balancing and prediction using graph methods
- AMR and unstructured grid parallelization
- VTK integration
- Hybrid messaging / threading parallel approaches
Recommended Reading

DIY

• Peterka, T., Ross, R.: Versatile Communication Algorithms for Data Analysis. 2012 EuroMPI Special Session on Improving MPI User and Developer Interaction IMUDI’12, Vienna, AT.

Particle Tracing Applications

Foundations of Data-Parallel Particle Advection

Thank You

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Subversion repositories
https://svn.mcs.anl.gov/repos/osuflow/trunk
https://svn.mcs.anl.gov/repos/diy/trunk

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