A Framework for Particle Advection for Very Large Data

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Advecting particles
Particle advection basics

Advection of particles create integral curves

\[ S'(t) = v(t, S(t)) \quad S(t_0) := x_0 \]

Streamlines: display particle path (instantaneous velocities)

Pathlines: display particle path (velocity field evolves as particle moves)
Particle advection is the duct tape of the visualization world. Advecting particles is essential to understanding flow and other phenomena (e.g. magnetic fields)!
Outline

- Efficient advection of particles
- A general system for particle-advection based analysis
Particle Advection Load Balancing

- N particles (P1, P2, … Pn), M MPI tasks (T1, …, Tm)
- Each particle takes a variable number of steps, S1, S2, … Sn
- Total number of steps is \( \sum S_i \)
  - We cannot do less work than this (\( \sum S_i \))
- Goal: Distribute the \( \sum S_i \) steps over M MPI tasks such that problem finishes in minimal time
Goal: Distribute the \( \sum Si \) steps over \( M \) MPI tasks such that problem finishes in minimal time

Sounds sort of like a bin-packing problem, but...
- particles can move from MPI task to MPI task
- path of particle is data dependent and unknown a priori (we don’t know Si beforehand)
- big data significantly complicates this picture....
  - ... data may not be readily available, introducing starvation
Advecting particles

What is the right strategy for getting particle and data together?

Decomposition of large data set into blocks on filesystem
Strategy: load blocks necessary for advection

Decomposition of large data set into blocks on filesystem

Go to filesystem and read block
Decomposition of large data set into blocks on filesystem

Strategy: load blocks necessary for advection

This strategy has multiple benefits:
1) Indifferent to data size: a serial program can process data of any size
2) Trivial parallelization (partition particles over processors)

BUT: redundant I/O (both over MPI tasks and within a task) is a significant problem.
“Parallelize over Particles”

- “Parallelize over Particles”: particles are partitioned over processors, blocks of data are loaded as needed.

- Some additional complexities:
  - Work for a given particle (i.e. Si) is variable and not known a priori: how to share load between processors dynamically?
  - More blocks than can be stored in memory: what is the best caching/purging strategy?
“Parallelize over data” strategy: parallelize over blocks and pass particles

This strategy has multiple benefits:
1) Ideal for in situ processing.
2) Only load data once.

BUT: starvation is a significant problem.
Both parallelization schemes have serious flaws.

- Two approaches:

<table>
<thead>
<tr>
<th>Parallelizing Over</th>
<th>I/O</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data</td>
<td>Good</td>
<td>Bad</td>
</tr>
<tr>
<td>Particles</td>
<td>Bad</td>
<td>Good</td>
</tr>
</tbody>
</table>

Hybrid algorithms
The master-slave algorithm is an example of a hybrid technique.

- Algorithm adapts during runtime to avoid pitfalls of parallelize-over-data and parallelize-over-particles.
  - Nice property for production visualization tools.
- Implemented inside VisIt visualization and analysis package.

Master-Slave Hybrid Algorithm

- Divide processors into groups of $N$
- Uniformly distribute seed points to each group

### Master:
- Monitor workload
- Make decisions to optimize resource utilization

### Slaves:
- Respond to commands from Master
- Report status when work complete
Master Process Pseudocode

```python
Master()
{
    while ( ! done )
    {
        if ( NewStatusFromAnySlave() )
        {
            commands = DetermineMostEfficientCommand()

            for cmd in commands
                SendCommandToSlaves( cmd )
        }
    }
}
```

What are the possible commands?
Commands that can be issued by master

1. Assign / Loaded Block
2. Assign / Unloaded Block
3. Handle OOB / Load
4. Handle OOB / Send

OOB = out of bounds

Slave is given a streamline that is contained in a block that is already loaded
Commands that can be issued by master

1. Assign / Loaded Block
2. Assign / Unloaded Block
3. Handle OOB / Load
4. Handle OOB / Send

OOB = out of bounds

Slave is given a streamline and loads the block
Slave is instructed to load a block. The streamline in that block can then be computed.
Commands that can be issued by master

1. Assign / Loaded Block
2. Assign / Unloaded Block
3. Handle OOB / Load
4. Handle OOB / Send

OOB = out of bounds

Slave is instructed to send a streamline to another slave that has loaded the block.
Master Process Pseudocode

Master()
{
    while ( ! done )
    {
        if ( NewStatusFromAnySlave() )
        {
            commands = DetermineMostEfficientCommand()
            for cmd in commands
                SendCommandToSlaves( cmd )
        }
    }
}

* See SC 09 paper for details
- When to pass and when to read?
- How to coordinate communication?
Status? Efficiently?

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Action</th>
</tr>
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<tr>
<td>0</td>
<td>T0 reads B0, T3 reads B1</td>
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Algorithm Test Cases

- Core collapse supernova simulation
- Magnetic confinement fusion simulation
- Hydraulic flow simulation
Workload distribution in parallelize-over-data

Starvation
Workload distribution in parallelize-over-particles

Too much I/O
Workload distribution in master-slave algorithm
Workload distribution in supernova simulation

Parallelization by:

Particles

Data

Hybrid

Colored by processor doing integration
Astrophysics Test Case:
Total time to compute 20,000 Streamlines

- **Uniform Seeding**
  - Data
  - Hybrid

- **Non-uniform Seeding**
  - Data
  - Hybrid

Graphs show the comparison of time taken (in seconds) for different numbers of processes (64, 128, 256, 512) for uniform and non-uniform seeding.
Astrophysics Test Case:
Number of blocks loaded

Uniform Seeding

Non-uniform Seeding

<table>
<thead>
<tr>
<th>Blocks loaded</th>
<th>64</th>
<th>128</th>
<th>256</th>
<th>512</th>
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<tbody>
<tr>
<td>Particles</td>
<td>500</td>
<td>1000</td>
<td>1500</td>
<td>2000</td>
</tr>
<tr>
<td>Data</td>
<td>100</td>
<td>200</td>
<td>300</td>
<td>400</td>
</tr>
<tr>
<td>Hybrid</td>
<td>150</td>
<td>300</td>
<td>450</td>
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Summary: Master-Slave Algorithm

- First ever attempt at a hybrid parallelization algorithm for particle advection
- Algorithm adapts during runtime to avoid pitfalls of parallelize-over-data and parallelize-over-particles.
  - Nice property for production visualization tools.
- Implemented inside VisIt visualization and analysis package.
Outline

- Efficient advection of particles
- A general system for particle-advection based analysis
Goal

- Efficient code for a variety of particle advection based techniques
- Cognizant of use cases with >>10K particles.
  - Need handling of every particle, every evaluation to be efficient.
- Want to support diverse flow techniques: flexibility/extensibility is key.
- Fit within data flow network design (i.e. a filter)
Motivating examples of system

- FTLE
- Stream surfaces
- Streamline
- Dynamical Systems (e.g. Poincaré Maps)
- Statistics based analysis
- + more
Design

- PICS filter: parallel integral curve system

Execution:

- Instantiate particles at seed locations
- Step particles to form integral curves
  - Analysis performed at each step
  - Termination criteria evaluated for each step
- When all integral curves have completed, create final output
Design

- Five major types of extensibility:
  - How to parallelize?
  - How do you evaluate velocity field?
  - How do you advect particles?
  - Initial particle locations?
  - How do you analyze the particle paths?
We disliked the “matching inheritance” scheme, but this achieved all of our design goals cleanly.
#1: How to parallelize?

- avtICAlgorithm
  - avtParDomIC-Algorithm (parallel over data)
  - avtSerialIC-Algorithm (parallel over seeds)
  - avtMasterSlaveICAlgorithm
#2: Evaluating velocity field

avtIVPField

- avtIVPVTKField
- avtIVPVTK-TimeVarying-Field
- avtIVPM3DC1 Field
- avtIVP-<YOUR>Higher Order-Field

IVP = initial value problem
#3: How do you advect particles?

IVP = initial value problem
#4: Initial particle locations

- avtPICSFilter::GetInitialLocations() = 0;
#5: How do you analyze particle path?

- `avtIntegralCurve::AnalyzeStep() = 0;`
  - All `AnalyzeStep` will evaluate termination criteria

- `avtPICSFilter::CreateIntegralCurveOutput(
  std::vector<avtIntegralCurve*> &) = 0;`

- **Examples:**
  - Streamline: store location and scalars for current step in data members
  - Poincare: store location for current step in data members
  - FTLE: only store location of final step, no-op for preceding steps

- **NOTE:** these derived types create very different types of outputs.
Putting it all together

Integral curves sent to other processors with some derived types of avtICAlgorithm.

PICS Filter

::CreateInitialLocations() = 0;

::AnalyzeStep() = 0;

Integral curves sent to other processors with some derived types of avtICAlgorithm.
VisIt is an open source, richly featured, turn-key application for large data.

- **Used by:**
  - Visualization experts
  - Simulation code developers
  - Simulation code consumers

- **Popular**
  - R&D 100 award in 2005
  - Used on many of the Top500
  - >>>100K downloads

217 pin reactor cooling simulation
Run on ¼ of Argonne BG/P
Image credit: Paul Fischer, ANL
Final thoughts...

- **Summary:**
  - Particle advection is important for understanding flow and efficiently parallelizing this computation is difficult.
  - We have developed a freely available system for doing this analysis for large data.

- **Documentation:**
  - (VisIt) [http://www.llnl.gov/visit](http://www.llnl.gov/visit)

- **Future work:**
  - UI extensions, including Python
  - Additional analysis techniques (FTLE & more)
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- **PICS framework**: Hank Childs (LBNL/UCD), Dave Pugmire (ORNL), Christoph Garth (Kaiserslautern), David Camp (LBNL/UCD), Allen Sanderson (Univ of Utah)
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