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In-Situ Interactive Visualization of HPC Simulations with Damaris

Joint work involving
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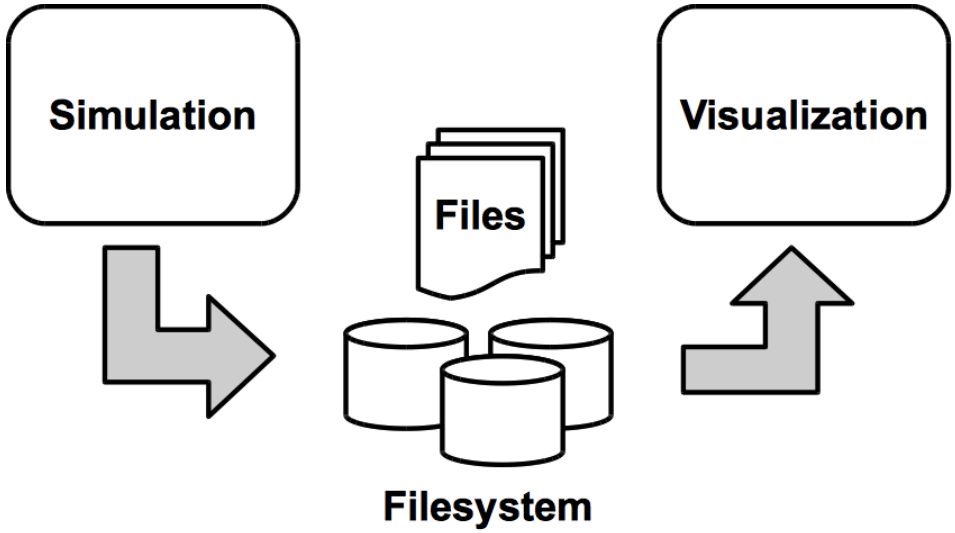
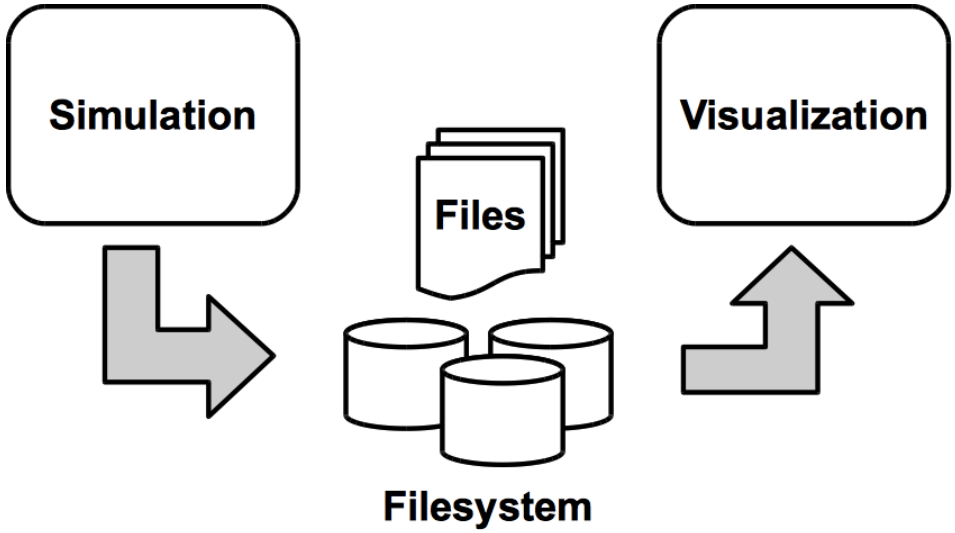
June 13th 2012

Introduction: when offline visualization does not work anymore…



- **The old fashioned way**
  - Offline visualization:
    - Run your simulation for days
    - Write a bunch of files periodically, using HDF5, NetCDF, etc.
    - Move the files to an analysis cluster
    - Analyze your data
    - ~~Find something scientifically relevant~~ notice the simulation didn't behave as expected

Introduction: when offline visualization does not work anymore…



- **Motivations**
  - I/O becoming a bottleneck: need to drastically reduce storage demands
  - Longer, more complex simulations: need to reduce the time-to-insight
  - Migrations of data to a visualization cluster become intractable
  - Visualization software also suffer from the I/O bottleneck
  - Need to adapt the output format from simulations to input readable from visualization

Towards inline visualization strategies

- **Loosely coupled strategy**
  - Visualization runs on a separate, remote set of resources
  - Partially or fully asynchronous
  - Solutions include staging areas, file format wrappers (HDF5 DSM, ADIOS, …)

- **Tightly coupled strategy**
  - Visualization is collocated with the simulation
  - Synchronous (time-partitioning): the simulation periodically stops
  - Solution by code instrumentation
  - Memory constrained

Four main goals

User friendliness

Low impact on simulation code

Adaptability
(to different simulations and visualization scenarios)

Performance

Low impact on simulation run time

Good resource utilization
(low memory footprint, use of GPU,…)

Driving the acceptance of any approach

Towards inline visualization strategies

Coupling		Tight	Loose	?
Impact on code		High	Low	Minimal
Adaptability	Interactivity	Yes	None	Yes
	Instrumentation	High	Low	Minimal
Impact on run time		High	Low	Minimal
Resource usage		Good	Non-optimal	Better

- Researchers seldom accept tightly-coupled in-situ visualization
  - Because of development overhead, performance impact…
  - "Users are stupid, greedy, lazy slobs" [1]
- **Is there a solution achieving all these goals?**

[1] D. Thompson, N. Fabian, K. Moreland, L. Ice, "Design issues for performing in-situ analysis of simulation data", Tech. Report, Sandia National Lab

Outline

- Introduction
- **In-situ capabilities in diverse software**
- Recall on the Damaris approach
- Using Damaris for in-situ visualization
- Conclusion

An overview of VisIt (LLNL)

- Provides the libsim library ➔ simulation instrumentation
- Data is exposed through a set of callback functions (in C or Fortran)
  - About 10 to 20 lines of code per variable/object to expose
  - Need to re-write the simulation's mainloop
- Works in a time-partitioning manner: simulation stops
  - If a user connected to the simulation ➔ interactively answers its requests
- Can work on data in memory without any copy

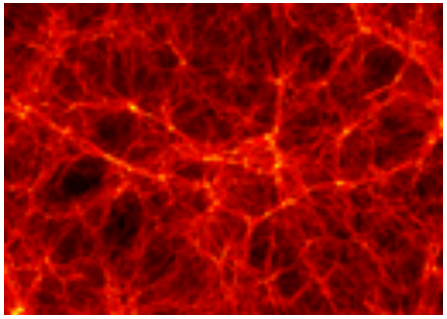
```
// This function is called to retrieve the mesh
visit_handle get_mesh_data(int domain, const char *name, void *cbdata) {
  visit_handle h = VISIT_INVALID_HANDLE;
  if(strcmp(name, "my_mesh") == 0) {
    if(VisIt_RectilinearMesh_alloc(&h) == VISIT_OKAY) {
      visit_handle hxc, hyc, hzc;
      VisIt_VariableData_alloc(&hxc);
      // ... idem for hyc and hzc
      VisIt_VariableData_setDataF(hxc, VISIT_OWNER_SIM, 1, NX, mesh_x);
      // ... idem for hyc and hzc
      VisIt_RectilinearMesh_setCoordsXYZ(h hxc,hyc,hzc);
      }
    }
    return h;
  }
}
```

Other visualization software

- ParaView
  - In-situ interface based on VTK, only available in C++
    - Not convenient for Fortran simulations
  - Fixed visualization pipeline, no interactivity
  - Possibility to write the visualization pipeline in Python
    - ParaView can generate a Python script from a user behavior
  - Possibility to redirect the output of the pipeline to a remote cluster (loosely coupled visualization capability)
- EzViz
  - Interface in C++ also, functionalities similar to ParaView
- …

The case of Enzo and YT (UCSD,…)

- **Enzo:** AMR astrophysical simulation developed by UC San Diego and other labs
- Has its own visualization system: **YT**, written in **Python** on top of **MatplotLib**
- **Enzo** wraps its data into **NumPy structures**, and periodically loads a user-provided Python script



Enzo is an example of simulation for which

- A specific visualization system has been designed
- A specific instrumentation has been done (using the Python/C interface)
- Yet the Enzo developers admit that time-partitioning is not appropriate [1], as it interrupts the simulation
- Moreover, loading Python modules have an increasing impact at large scale [2]

[1] "YT: A multi-code analysis toolkit for astrophysical simulation data", M. J. Turk, B. D. Smith, J. S. Oishi, S. Skory, S. W. Skillman, T. Abel, M. L Norman, in The astrophysical journal supplement series, January 2011

[2] Personal experiments on JaguarPF, and private discussions with J. M. Favre

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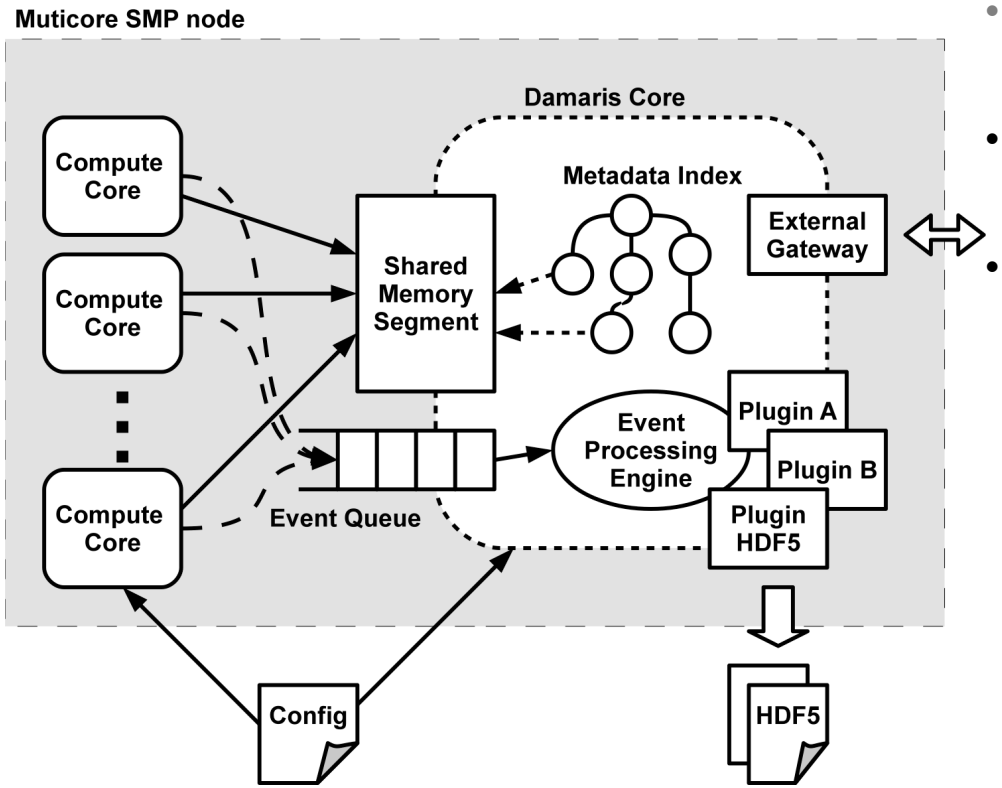
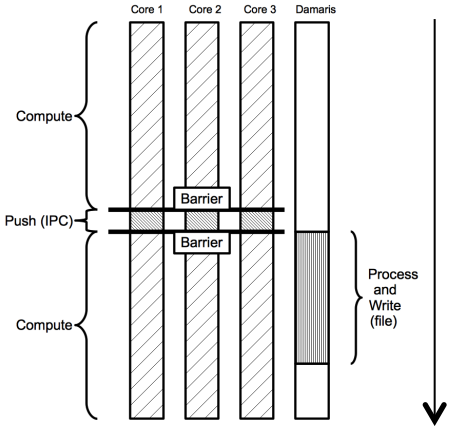
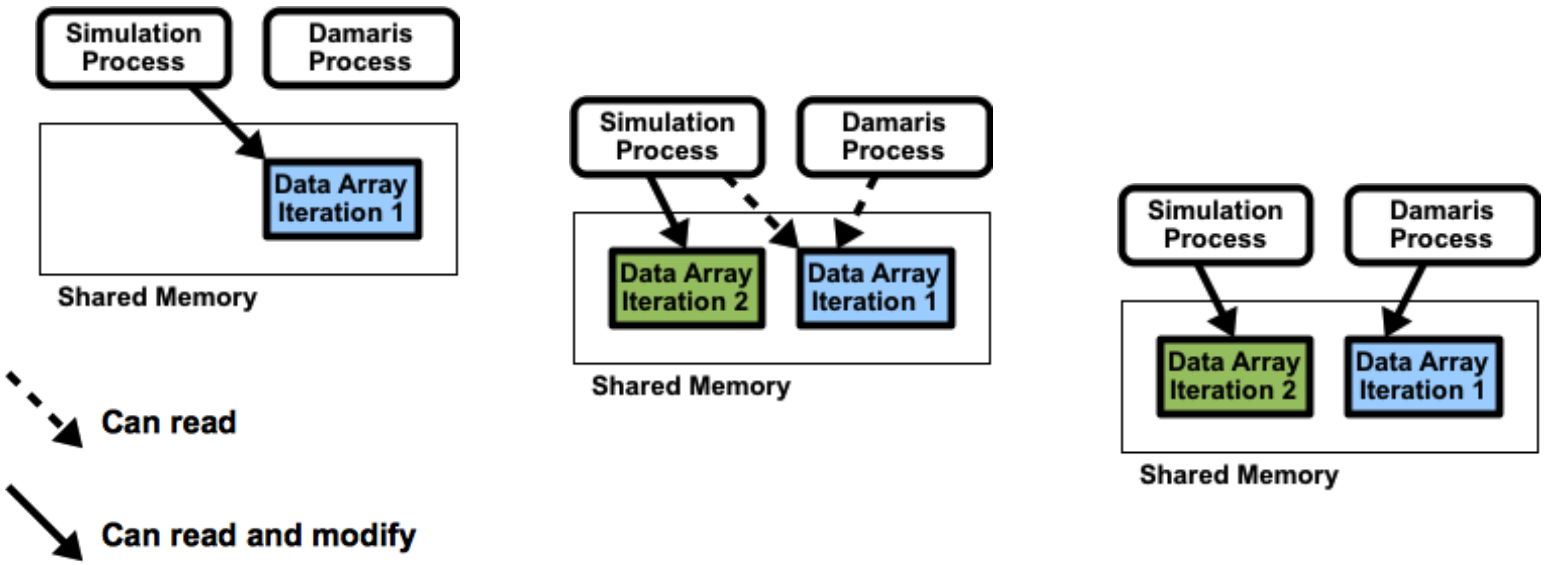
Damaris at a glance



- *Dedicated Adaptable Middleware for Application Resources Inline Steering*
- **Main idea:** dedicate one or a few cores in each SMP node for data management
- **Features:**
  - Shared-memory-based communications
  - Plugin system (C,C++, Python)
  - XML external description of data

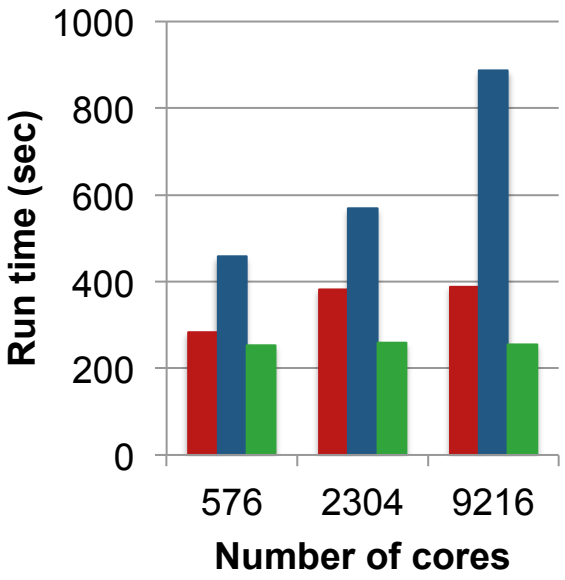


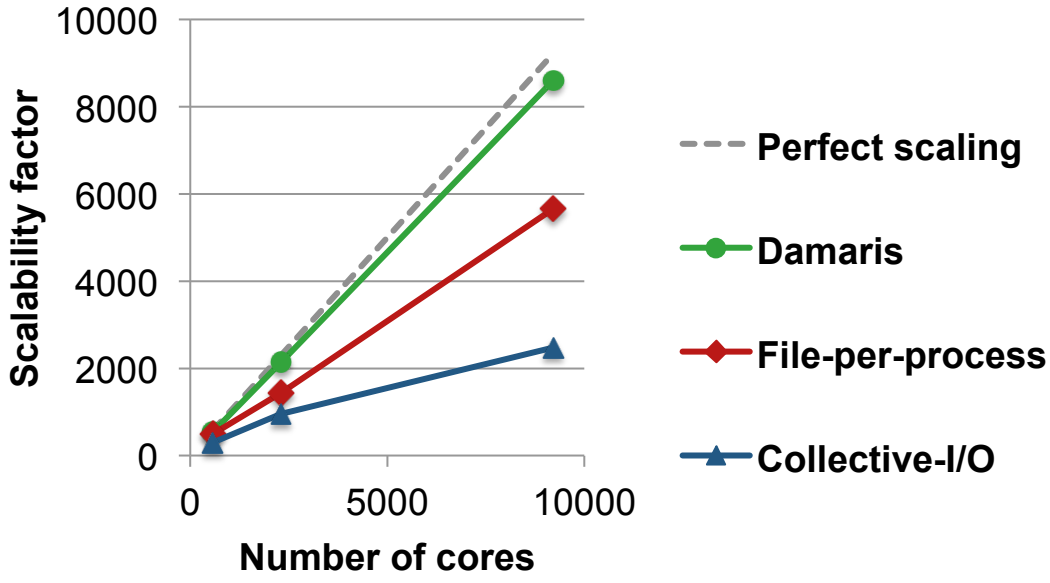
Damaris: efficiently leveraging shared-memory



- Two versions of the data
- Direct allocation in shared-memory
  - DC_alloc("varname",iteration)
- Overlap read-access on past iterations
- Avoids copy of data

Results on I/O with the CM1 application
Damaris achieves almost perfect scalability

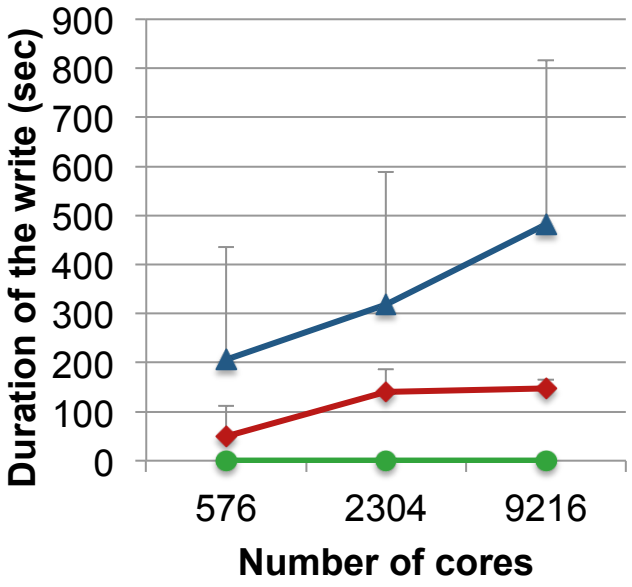




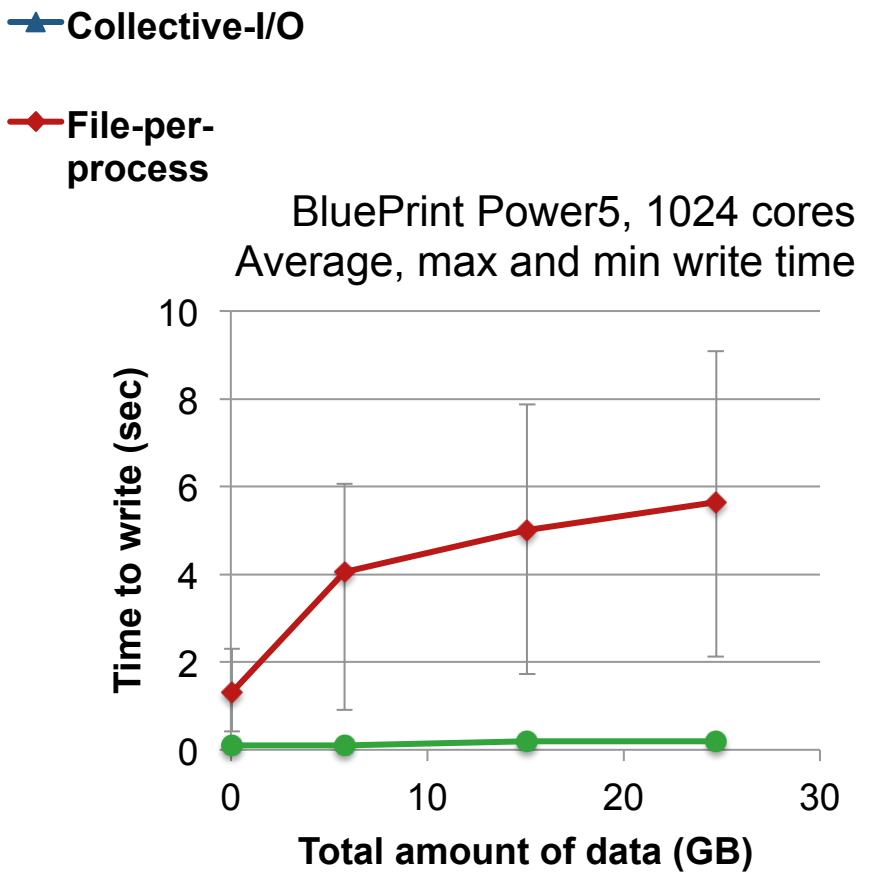
Weak scalability factor $S = N \frac{T_{base}}{T}$

N: number of cores
$\mathbf{T_{base}}$: time of an iteration on one core w/ write
T: time of an iteration + a write

Results on I/O with the CM1 application
Damaris hides the I/O jitter

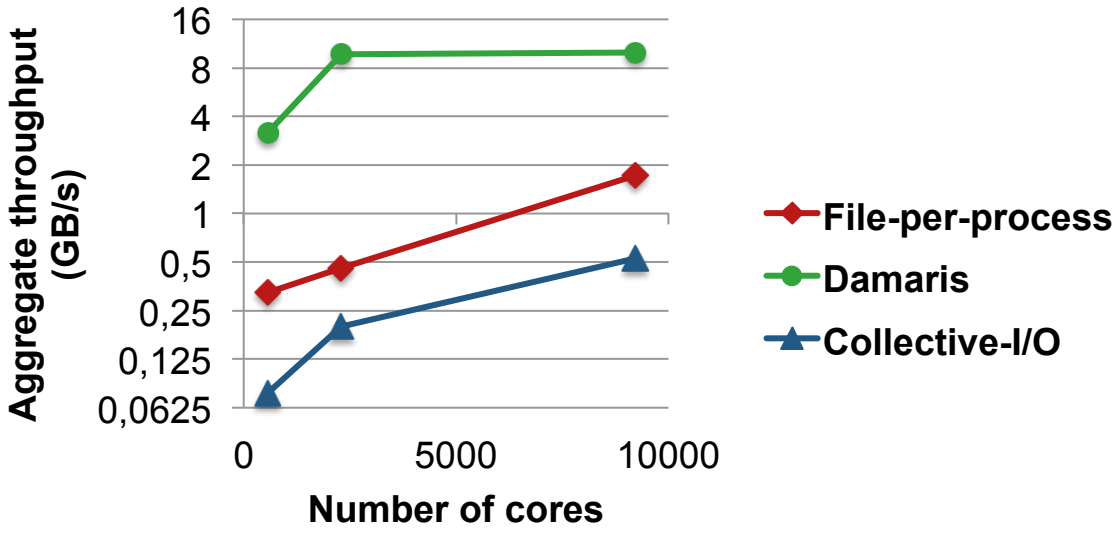


Kraken Cray XT5
Average and maximum write time
28MB per process



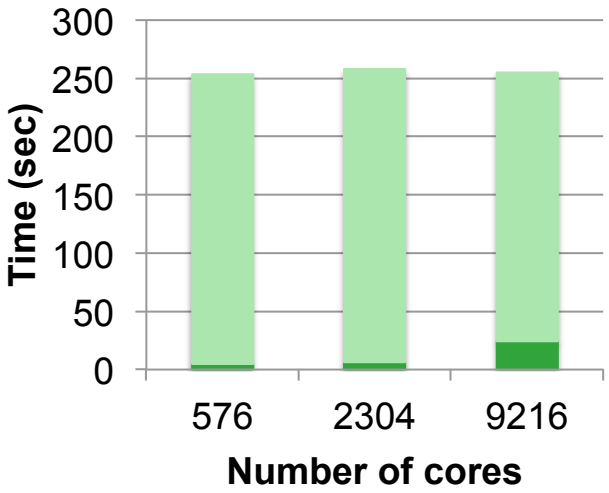
Results on I/O with the CM1 application
Damaris increases effective throughput

Average aggregate throughput from the writer processes



Results on I/O with the CM1 application

Time spent by Damaris writing data and time spent waiting



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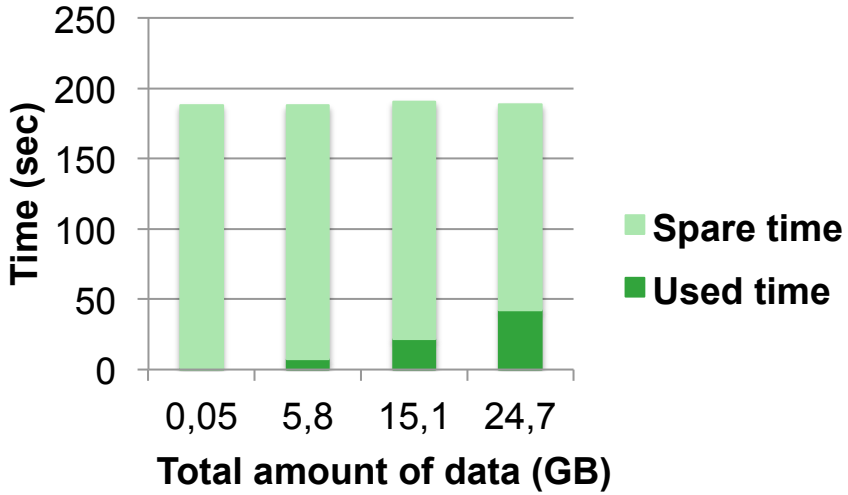

BluePrint Power5 (1024 cores)

Damaris spares time?
Let's use it for visualization!

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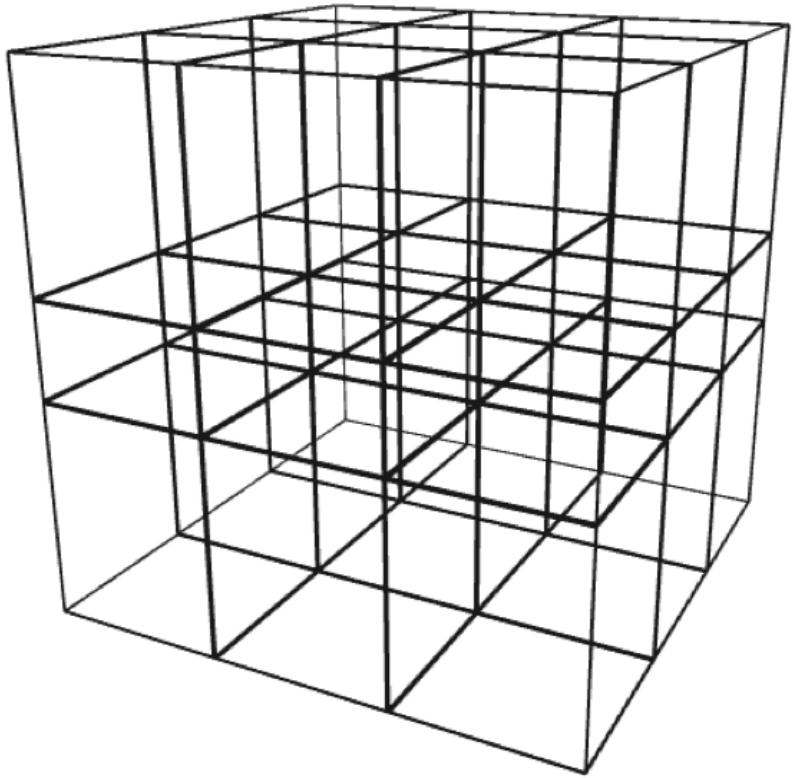
Let's take a representative example



```
// rectilinear grid coordinates
float mesh_x[NX];
float mesh_y[NY];
float mesh_z[NZ];
// temperature field
double temperature[NX][NY][NZ];
```

“Instrumenting” with Damaris

```
DC_write(“mesh_x”,iteration,mesh_x);
DC_write(“mesh_y”,iteration,mesh_x);
DC_write(“mesh_z”,iteration,mesh_x);

DC_write(“temperature”,iteration,temperature);
```

(Yes, that’s all)

Now describe your data in an XML file

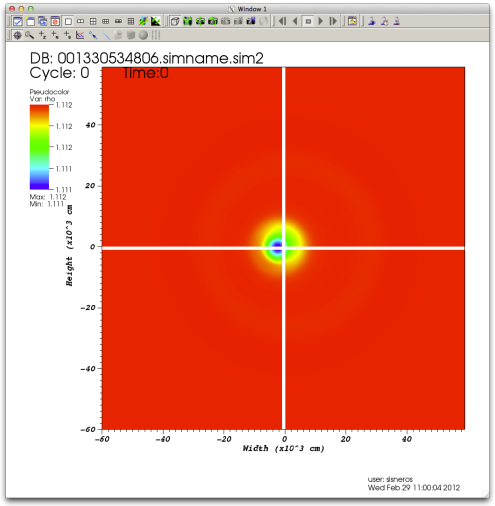
```
<parameter name="NX" type="int" value="4"/>
<layout name="px" type="float" dimensions="NX"/>
<variable name="mesh_x" layout="px">
<!-- idem for PTY and PTZ, py and pz, mesh_y and mesh_z -->

<layout name="data_layout" type="double" dimensions="NX,NY,NZ"/>
<variable name="temperature" layout="data_layout" mesh="my_mesh" />

<mesh type="rectilinear" name="my_mesh" topology="3">
   <coord name="mesh_x" unit="cm" label="width" />
   <coord name="mesh_y" unit="cm" label="depth" />
   <coord name="mesh_z" unit="cm" label="height" />
</mesh>
```

- Unified data description for different visualization software
- Damaris translates this description into the right function calls to any such software (right now: Python and VisIt)
- Damaris handles the interactivity by synchronizing and un-synchronizing dedicated cores

Using Damaris plugins system



- Plugins can be written in C, C++ or Python
- Very simple API from the simulation:
  - `DC_signal("event_name",iteration)`
- Different scopes of event: core, node, global
- Events are also exposed to VisIt: users can trigger an event himself from VisIt's interface ➔ enhanced interactivity

```
var = damaris.open("temperature")
for chunks in var.select( iteration = 1 )
        print numpy.average(chunks.data)
```

- Plugin system already used to implement an HDF5 persistency layer
- Connection between VisIt and Damaris was initially implemented as a plugin written by Roberto Sisneros (NCSA): very good feedback on usability
  - Now fully integrated within Damaris
- New challenge rising with Python: loading modules from many cores, doesn't scale

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Conclusion:
Using Damaris for in-situ visualization

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Impact on code		High	Low	Minimal
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	Instrumentation	High	Low	Minimal
Impact on run time		High	Low	Minimal
Resource usage		Good	Non-optimal	Better

- Impact on code: 1 line per object (variable or event)
- Adaptability to multiple visualization software (Python, VisIt, ParaView, etc.)
  - Plugins, XML
- Interactivity through VisIt
- Impact on run time: simulation run time independent of visualization
- Resources usage:
  - preserves the "zero-copy" capability of VisIt thanks to shared-memory,
  - can asynchronously use GPU attached to Cray XK6 nodes

thank you!