A Maya Use Case: Adaptable Scientific Workflows with ADIOS for General Relativistic Astrophysics

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Outline

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Numerical Relativistic Simulations with Maya  
Maya Code  
Data Processing and Analysis

Our Approach to Maya Workflow Improvement  
Incorporating ADIOS into Maya as Fast I/O System

Incorporating ADIOS into Maya  
Magneto-hydrodynamics  
Particles

How to Make Maya Simulations Interactive and Steerable at Runtime  
Exploiting Flexpath/ADIOS in Maya

Summary
Maya-RDAV Introduction

High-level Research Goals

- Enrich runtime for, and user’s experience with, numerical relativistic (NR) simulations
- Provide apparatus for monitoring and interactive steering to astrophysics simulations at runtime
- Target XSEDE HPC and visualization systems to allow the user to connect Kraken, Keeneland, and Nautilus

- Collaboration effort: active computational astrophysics and computer science
- Part of RDAV (Remote Data Analysis and Visualization) project
Maya Code

- 3D numerical relativistic calculations simulating creation and collision of black holes
- Solves Einstein’s equations for black holes, stars, etc
- Based on Einstein Toolkit, Cactus, and Kranc; uses Carpet AMR module
- Uses Georgia Tech’s custom spacetime and hydrodynamics evolution code
Maya Workflow

**Data Factory**
- Maya Simulation
  - ADIOS Thorn
  - Stage Area
  - Parallel Storage

**Importing/Exporting Raw Data**
- User
  - Submit runview job
  - Run periodically

**Data Processing**
- User
  - Browse, check, if correct, etc; stop simulation if catastrophic
  - Run summary.sh
  - Generate processed data
  - Run h5movie.sh
  - Run ADIOSBPmovie.sh
  - Run CarpetIO plugin
  - Run Visit

**Data Visualization**
- Website publish
  - http://numrel.org

**Summary directory:** contains .png, .html, movies etc

**Control path**
- Data path
- Data processing
Data Processing and Analysis in Maya

Data

- Physical quantities of interest, e.g., matter density, magnetic field components, gravitational radiation intensity
- Periodic checkpoints

Processing and analysis

- Some physical quantities scrutinized during in-simulation analysis (analysis thorns)
- Post-processing including interactive analysis, scripted plots, and movies
Maya I/O Characteristics and Challenges

- Expensive I/O: assumption of keeping I/O overhead at 40% of walltime → write out a small number of variables with a lower dimensionality
- Mostly static, shell-based, post-processing-based data analysis and visualization
- A typical simulation:
  - A couple of weeks on a local cluster
  - Recording 15 2D physical variables of interest
  - 21GB output data (15 3D variables would generate 4.5TB)
  - Utilize a combination of HDF5 and ASCII for writes

As a consequence

- Not all variables get written out. Experimenters pre-select a small subset for each run
- Requires reruns of the simulations if correct variables were not output
- Simulation data sets prone to corruptions with large files
Our Approach to Maya Workflow Improvement

- Incorporating new staging I/O technologies to reduce I/O overhead
  - Enable outputting more physical variables of interest
  - Enable outputting higher dimensionality of variables
- Expanding the existing Maya workflow to address inline visualization and steering
ADIOS – Adaptable I/O System as Our Fast I/O

- A componentization of the I/O layer with a selection of various I/O methods
- Designed to provide a scalable, portable, and efficient I/O solution for various computer infrastructures
- In certain cases demonstrated I/O performance improvements of factor 1000 over established parallel file formats
- Successfully incorporated into several scientific codes including GTC fusion code, GTS, Chimera, XGC0, XGC1, Flash, S3D
Advantages of Using ADIOS

- Ease switching to other transport method (MPI, MPI_AMR, Flexpath, etc)
- Offers memory-to-memory coupling solutions (Flexpath)
- Self-describing BP file format
  - Ability to avoid runtime costs related to file consistency validation
  - Footer index—does not necessitate moving it whenever data length change occurs
  - Resilience support
- More info

www.olcf.ornl.gov/center-projects/adios/
How to Improve Maya Workflow with ADIOS

Data Factory

Maya Simulation

ADIOS Thorn

Stage Area

Parallel Storage

Importing/Exporting
Raw Data

User

cron

run periodically

runview.sh

Data Processing

Browse, check, if correct, etc; stop simulation if catastrophic

processed data

Python script

generate

movie frames

Visit

run- summary.sh

h5movie.sh

2d hdf5 data

run- control

Data Visualization

Website publish

http://numrel.org

Summary directory:
contains .png, .ht ml, movies etc

Simulation Machine

Data Processing Nodes

Control path

Others

Data path

Data processing
Incorporating ADIOS into Maya: CarpetIOADIOS Thorn
Magneto-hydrodynamics simulations

- Early prototype demonstrated an improvement in output performance from 3-5 minutes for a full I/O checkpoint using HDF5 to 6 seconds using ADIOS on Kraken
- After a number of tuning operations on NICS machines, the equivalent HDF5 runs take 15 secs on Kraken
- This is still a 60% improvement in output performance
- Hopefully, the CarpetIOADIOS thorn will be released in a couple of months
Incorporating ADIOS into Maya: Particles

Particle-based simulations

- Early prototype shows 35% improvement over standard I/O methods in the simulation of 1 million particles running on 192 threads with 8 OpenMP threads per MPI process.

- Ease of adding ADIOS support to particle based simulations (one afternoon + accelerators ;)

![Simulation Image]
Incorporating ADIOS into Maya: Current Progress

- Due to recent change in ADIOS API, we had to modify our ADIOS-based checkpoint file format
- Validating the new file format
  - Debugging and performance evaluation of the newest CarpetIOADIOS thorn on Kraken and Nautilus
Exploiting Flexpath – ADIOS Transport Method – in Maya

- Included in ADIOS spec and distribution
- One of standard ADIOS transport methods – switching to Flexpath is easy:

```c
// config.xml
<method group="temperature" method="FLEXPATH">QUEUE_SIZE=4;</method>

// writer
adios_init ("config.xml", comm);

// reader
adios_read_init_method(ADIOS_READ_METHOD_FLEXPATH, comm, "");
ADIOS_FILE* afile = adios_read_open("config.xml",
   ADIOS_READ_METHOD_FLEXPATH, comm, ADIOS_LOCKMODE_NONE, 0.0);
.....
adios_read_finalize_method(ADIOS_READ_METHOD_FLEXPATH);
```

Advantages of using Flexpath

- Will allow to gain on-demand insights into simulations at runtime
- Will offer dynamic exploration of data
- Fast I/O and binary filtering will enable the scientist to formulate very specific queries related to NR systems being evolved
Flexpath Technical Details

- Provides memory-to-memory coupling
- Allows for memory-to-disk and disk-to-memory operations using efficient buffered I/O in the staging area (as part of ADIOS)
- An event-based method (EVPath) with inline transformation support
- Uses in-system JIT compiler to deploy binary filters at runtime
- Offers multi-protocol overlay networking, including multi-machine, advanced shared memory support, networking over RDMA (Remote Direct Memory Access)
Summary

- **Maya-RDAV project**
  - Enrich runtime for numerical relativistic simulations and allow physicists to interactively monitor and steer computations at runtime

- **Approach**
  - Improve Maya workflow by incorporating ADIOS

- **Implementation**
  - Cataloged existing Maya workflow
  - ADIOS integration: Carpet I/O thorn + VisIt ADIOS plugins for (magneto-)hydrodynamics and particle-based NR simulations
  - Flexpath: providing memory-to-memory coupling + advanced binary filtering to enable dynamic exploration of data
Acknowledgments

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Future Work

- Performing more aggressive analytics with large datasets
- Reslicing data across all space-time
- Adding HTML5 extensions to the existing workflow

THANK YOU