

Scientific Simulation Analysis in Mathematica: Computable Data from Simulations

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Introducing SimulationTools

- A free software package for the analysis of numerical simulation data in Mathematica.
- Functional interface to your simulation



- Used daily for science - heavily optimised for performance
- Generic and modular - can be extended to support different codes

Design Principles

- Clean high-level interface hide low-level technical details
- Follow Mathematica **conventions** wherever possible
- Consistency and simplicity
- Extensible
- General
- Use domain language of the user, not of the implementation:
 - ReadBHCoordinates["mysim"]

not

Import["/simulations/mysim/output-0000/
tracker0.asc","Table"][[All, {1,5}]]

Design



Wednesday, 18 January 2012

Data Representations



- List with coordinates
- Introduce a new Mathematica type

000	IMS notebook	0
In[200]:=	data1 = MakeDataTable[data1]	רנ 🌔
Out[200]=	DataTable[]	Ę
In[201]:=	data2 = MakeDataTable[data2]	3]
Out[201]=	DataTable[]	Ę
In[203]:=	datal + data2 // ToList	3]
Out[203]=	{{0.,200}, {0.1,400}, {0.2,300}}	9]
In[204]:=	Sin[data1] // ToList	ן נ
Out[204]=	{{0., Sin[100]}, {0.1, Sin[200]}, {0.2, Sin[150]}}	
	150%	

Heavyweight data import

- Terabytes of 3D HDF5 files
- Import reads HDF5:
 - Separate files: one per supercomputer process (efficiency)
 - Adaptive mesh refinement
- NRMMA Cactus file reader: high-level interface to variables in a simulation



Extensible and optimised

Visualisation and Analysis

- Once data is in Mathematica, you can do anything!
 - Basic algebraic operations
 - Any Mathematica function can be mapped over data variables (cf. Map, MapThread)
 - Interpolation to get continuous functions rather than list data
 - Line/surface integrals
 - Plotting, movies,
 Manipulate



Remote Visualisation

- Large data on remote supercomputer
- Mathematica remote kernels:
 - Notebook frontend on laptop/ workstation
 - Kernel on remote machine
- Caveats:
 - Requires Mathematica (and licence) on supercomputer
 - Local notebook interface very sensitive to remote kernel hang (save often!)



Chunking

- Supercomputers **restrict time** for each job to ~24 hours
- Long-running simulations are split into **chunks** (checkpoint+recovery)
- NRMMA:
 - Internal routines combine chunks automatically
 - User never needs to know about simulation chunking
 - Applies to all file access in NRMMA

Examples: Simulation Overview

In[218]:= SimView["bbh"]



bbh





Re[Psi422], R = 100.



	Simulation	Cores	CPU hrs.	Davs	CPU	hrs./day	Estimated	finis	3h
w	bbh	12	0.343991	0.00119441		288 F	ri 30 Mar 20	12 13:	24:16
		Simula	ation			Segme	nts		
				Segment	:	Last output		t1	t2
50 300		bb	h	0000		Fri 30 Mar 20	12 13:24:13	0	6.5
				0001		Fri 30 Mar 201	12 13:24:16	7	300

Examples: Expressions on Data

000	IMS notebook (kop)	\bigcirc
(kop) In[1]		^ (
	<< nrmma	1
(kop) In[65	j:=	Y
	<pre>run = "/lustre/datura/rezzolla/MBNSs_vecpot/Meudon-MHD-moving-45km_noexcise_dx0.15</pre>	
	_Centered_Binatmo_ModifiedID_BIeI2_IF_PPM_whiskydiss0.1_fluxCD/hdf5";	1
(kop) In[38	3]:=	9
	rl = 5; it = 10240;	
(kop) In[74]:=	11
	<pre>rho = ReadGridFunction[run, "rho.xz.h5", it, rl]</pre>	
(kop) Out[2
	DataRegion[HYDROBASE::rho, {101, 96}, { $(-0.45, 14.55)$, { $-0.45, 13.8$ }]	11
(kop) In[78	5]:=	91
	<pre>v = Map[ReadGridFunction[run, # <> ".xz.h5", it, rl] &, {"vel[0]", "vel[1]", "vel[2]"}]</pre>	
(kop) Out[75]=	٩
	{DataRegion[HYDROBASE::vel[0], {101, 96}, {{-0.45, 14.55}, {-0.45, 13.8}]],	
	DataRegion[HYDROBASE::vel[1], {101, 96}, {{-0.45, 14.55}, {-0.45, 13.8}}],	
	DataRegion[HIDROBASE::Vel[2], {101, 90;, $\{\{-0.45, 14.55\}, \{-0.45, 15.0\}\}$]	''U
(kop) ln[76	b]:=	91
	<pre>B = Map[ReadGridFunction[run, # <> ".xz.h5", it, rl] &, {"Bx", "By", "Bz"}]</pre>	
(kop) Out[76]=	7
	{DataRegion[WHISKY::Bx, {101, 96}, {{-0.45, 14.55}, {-0.45, 13.8}}],	
	DataRegion[WHISKY::By, {101, 96;, {{-0.45, 14.55}, {-0.45, 13.8}}], DataRegion[WHICKY::Bz, {101, 96;, {{-0.45, 14.55}, {-0.45, 13.8}}],	
	Datakegion[whi5Ki::BZ, {IUI, 90;, {{-0.45, 14.55}, {-0.45, 13.8}}]}	11

Examples: Expressions on Data

000	MS notebook (kop)	0
	<pre>x = GetCoordinate[rho, 1]</pre>	ןנ ו
	DataRegion[HYDROBASE::rho, {101, 96}, {{-0.45, 14.55}, {-0.45, 13.8}}]	Ϊ
	<pre>z = GetCoordinate[rho, 2]</pre>	J
	$\texttt{DataRegion[HYDROBASE::rho, \{101, 96\}, \{\{-0.45, 14.55\}, \{-0.45, 13.8\}\}]}$	
	er = {x, 0., z} / Sqrt [$x^2 + z^2$]	ןנ
	<pre>{DataRegion[HYDROBASE::rho, {101, 96}, {{-0.45, 14.55}, {-0.45, 13.8}}], DataRegion[HYDROBASE::rho, {101, 96}, {{-0.45, 14.55}, {-0.45, 13.8}}], DataRegion[HYDROBASE::rho, {101, 96}, {{-0.45, 14.55}, {-0.45, 13.8}}]</pre>	
	Sr = (B.Bv - Bv.B).er	3]
	DataRegion[HYDROBASE::rho, {101, 96}, {{-0.45, 14.55}, {-0.45, 13.8}}]	
	Max[Sr]	ןנ
	3.09023×10^{-20}	J D
	Min[Sr]	ןנ
	-8.2132×10^{-21}	<u>م</u>
	150% ► ◄) • //

Examples: Expressions on Data

- Make movies of derived variables
- Do any other analysis
 needed



Examples: Falloff of gravitational field

- Measure how gravitational field behaves along outgoing radial light paths
- For each iteration, have 1D simulation output data (HDF5)
- Read these into Mathematica (ReadGridFunction):
 - Compute light paths
 - Interpolate gravitational field onto them
 - Measure falloff of field along light paths (FindFit)
- Consistent with previously disputed theorem of Sachs, Newman and Penrose [Hinder et al, 2011]



Development/Quality

- **Documented** (usage messages, examples, tutorials)
- Unit tests
- Developed in package (.m) files for easy version control
- BitBucket project-hosting

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nmma is a Mathe	matica package for the	e analysis of data in Numerical I	Relativity		
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Enhancements to Mathematica

- Detected error conditions in NRMMA are reported via exceptions: computations do not continue uselessly
- Uncaught exceptions give stack backtraces; helps in debugging
- Warnings for assignments to undeclared variables
- Our own custom HDF5 reader mostly compatible with built-in Import
 - Avoid memory leaks and crashes when Import used with very large HDF5 data
 - Available already: <u>http://sourceforge.net/p/h5mma/</u>

Summary and Future Plans

- Functional interface to simulation data
- Highly-optimised data readers for Cactus code; additional readers possible
- Bring all the **power of Mathematica** to your simulation analysis!
- Planned:
 - Public release (GPL) [still polishing!]
 - Think of a better name
 - Remote data access at HDF5 level; avoid need for remote kernel on supercomputer
 - Transparent handling of **mesh-refined** data grid as an object