The Cactus Framework

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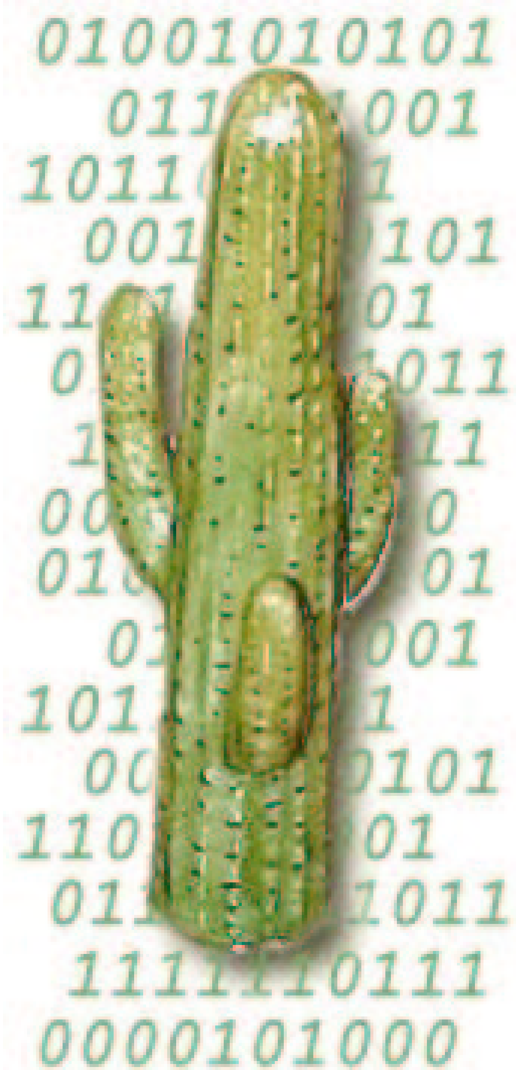
Outline

- History
- The Cactus User Community
- Cactus
- Usage Patterns

Bird's eye view

- Cactus is a freely available, portable, and manageable environment for collaboratively developing parallel, scalable, high-performance multi-dimensional component-based simulations

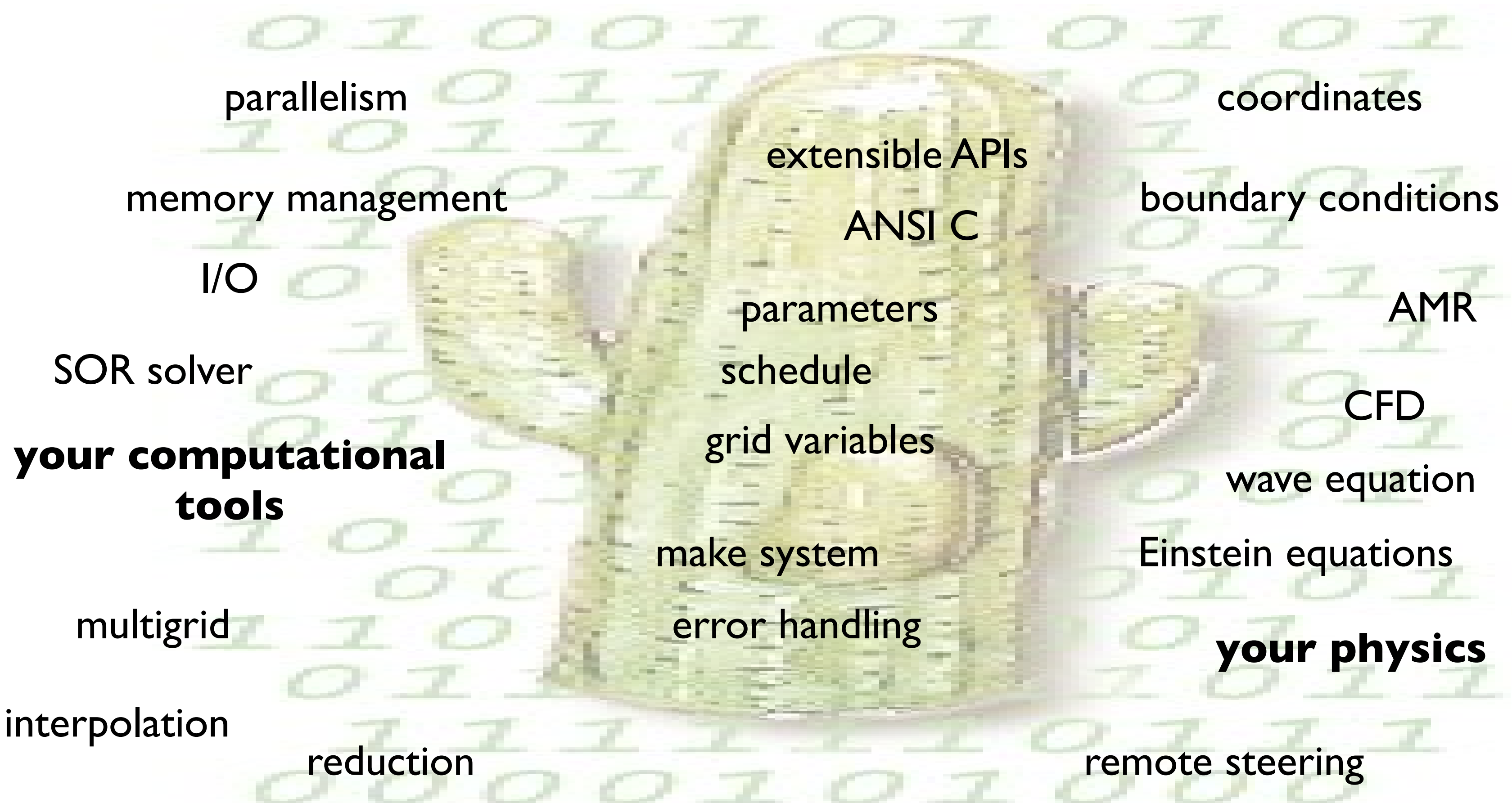


Saguaro
(Carnegiea gigantea)

History

- Cactus 1.0 was released in April 1997 at NCSA by the numerical relativity group
- Cactus 4.0 is available since 1999
- Since then incremental (i.e., mostly backwards-compatible)development
- Most users today still in numerical relativity

Overall Design



Core *flesh* with plug-in *thorns*

User Base

- Some groups base their whole code on Cactus
- Some groups use Cactus on the side
- In some places, individual students/postdocs use a Cactus-based public code
- Most Cactus users write thorns
- Few Cactus users contribute to the infrastructure
- Cactus and the core thorns are public (LGPL)
- Many thorns are private

Development Process

- Flesh and core thorns are developed by a small group
- Weekly video conferences
- Frequent bug reports/ feature requests from users
- Trying to balance stability and new features
- Mostly steady development with ~10 releases; many users live off CVS, not stable versions
- (Physics thorns are developed by physicists)

Einstein Toolkit

- A common infrastructure for all relativity codes
- Defines common variables, common schedule events, etc.
- Comes with public thorns for basic tasks (simple initial data, simple analysis methods)
- There are least five production level relativity codes based on Cactus, all but one private, all using the Einstein Toolkit
- Three-level structure:

Physics code

Einstein Toolkit

Computational Toolkit

Library vs. Framework

- A framework is like a library, except that it contains the main programme -- the user modules are libraries

- Crucial for easy interoperability -- otherwise, two modules may "fight" over who may be the main programme

- Cactus thorns are "connected" via their schedule

- Schedule is constructed at run time -- no code needs to know all compiled thorns

- Thorns can be developed completely independently

Anatomy of a Thorn

- A thorn in Cactus contains:
  - Cactus declarations (CCL language)
  - source code (C, C++, Fortran)
  - makefile fragments
  - documentation
  - test cases
  - example parameter files
- Thorns are the basic modular units
- Usually, each thorn is in a separate CVS repository

interface.ccl

- Declares *thorn name* and *implementation name*
- Declares *grid functions*
- Can *inherit* public grid functions from other implementations
- Declares *routines* (APIs provided/used by the thorn)

```
IMPLEMENTS: ADMConstraints
INHERITS: ADMBase

CCTK_REAL Hamiltonian TYPE=gf
{
  ham
} “Hamiltonian Constraint”

CCTK_REAL Momentum TYPE=gf
{
  momx momy momz
} “Momentum Constraint”
```

schedule.ccl

- Calls routines at certain times, e.g. *initial* or *evol* or *analysis*
- *Schedule groups* introduce a hierarchical structure
- Rule-based: schedule *AFTER*, *BEFORE*, *WHILE*
- Allocates storage for grid variables
- Synchronises variables

```
SCHEDULE ADMConstraints_Calculate AT analysis
{
  LANG: Fortran
  STORAGE: Hamiltonian Momentum
  SYNC: Hamiltonian Momentum
  TRIGGERS: Hamiltonian Momentum
} "Calculate the constraints"
```

param.ccl

- Declares parameters
- Five types: integer, real, boolean, keyword, string
- Allowed ranges need to be declared
- Can “inherit” public parameters from other implementations, possibly extending ranges

```
SHARES: ADMBase

EXTENTS KEYWORD initial_data
{
  “gaussian” :: “Gaussian pulse”
}

PRIVATE:

CCTK_REAL gaussian_amplitude \
  “Amplitude”
{
  0.0:* :: “must be nonnegative”
} 1.0
```

Example Source Code

```
#include "cctk.h"
#include "cctk_Arguments.h"

subroutine ADMConstraints_calculate (CCTK_ARGUMENTS)
  implicit none
  DECLARE_CCTK_ARGUMENTS

  CCTK_REAL :: dx, dy, dz
  integer   :: i, j, k

  dx = CCTK_DELTA_SPACE(1)
  ...

  do i = 2, cctk_lsh(1)-1
    ...
    ham(i,j,k) = (gxx(i+1,j,k) - gxx(i-1,j,k)) / (2*dx)
    ...
```

Parameter Files

- At run time, parameter files activate thorns and specify parameter values
- Not all compiled thorns need to be active

```
ActiveThorns = “PUGH CartGrid3D ADMBase IDSimple ADMConstraints”

driver::global_nx = 101
...
grid::xmin =  0.0
grid::xmax = 30.0
...
grid::type = “octant”

ADMBase::initial_data = “Minkowski”
```

Driver

- A *driver* is a special thorn that handles memory management and parallelisation
- Two drivers exist: *PUGH* (uniform grid) and *Carpet* (AMR, multi-block)
- Two more AMR drivers in development, based on *SAMRAI* and *Paramesh*
- Interpolation, reduction, and hyperslabbing operations closely tied to driver
- I/O (efficient and parallel) and checkpointing/recovery also somewhat driver specific

Application Base

- Current Cactus users are mostly in numerical relativity, including relativistic hydro
- We begin to use it for CFD
- Sporadic uses in many fields: astrophysics (Zeus), chemistry, oil field simulations, ...
- Cactus is mostly used for 3D time evolution with explicit time stepping
- Non-trivial initial data (elliptic equations) are mostly imported (this used to be different)
- We have a few public “Killer Thorns”

Visualisation

- gnuplot, xgraph, ygraph, etc. for 1D and 2D ASCII output
- Common HDF5 data format for Cactus simulations (because I/O is from a few thorns only)
- Amira, OpenDX for both debugging and production visualisation
- Built-in web server with jpeg slides
- www.cactuscode.org:5555/

Metadata and Data Preservation

- Thorn *Formaline* collects meta-data about a simulation (and sends them to a server)
- Collects machine name, user name, parameters, current simulation time, special events, etc.
- Allows real-time overview about currently running simulations by all people on all machines
- Some simulation results are later semi-automatically staged to be permanently stored in an archive

Discretisations

- Cactus supports block-structured regular grids best
- We use both Berger-Oliger AMR and multi-block discretisations
- We use (high order) finite differences
- Some experiments with pseudo-spectral discretisations
- Some experiments with particle codes (SPH)
- Plans for unstructured grids (finite elements, finite volumes)

Performance

- Performance must be measured
- Parallelisation performance depends on driver thorn
- I/O performance depends on I/O thorns
- Important: convenient pervasive performance measurements for application code
- Cactus offers timers
- Automatic timers for each scheduled routine

Random Details

- CCL files are parsed by perl code, creating C code and latex files
- Makefile fragments require GNU make
- Flesh written in ANSI C, thorns can be C, C++, or Fortran; other languages could be "easily" added
- Flesh helps with function calls between different languages (strings!)
- Fortran code is preprocessed with cpp (and sanitised with perl)
- Documentation uses latex

Building Cactus

- User can build several different *configurations* in the same Cactus tree
- User chooses list of thorns and set of options for each configuration
- Cactus is not "installed" in the way e.g. PETSc is; each user has the complete source tree
- Problem: User makes private modification → user forgets → results are not reproducible (solution: store source for each simulation)
- We keep a list of known good build options for each machine

Further Information

- Cactus: www.cactuscode.org
- Live simulation: www.cactuscode.org:5555
- Carpet (AMR driver): www.carpetcode.org
- Goodale et al., "The Cactus Framework and Toolkit: Design and Applications", Vector and Parallel Processing - VECPAR'2002, Lecture Notes in Computer Science