Cactus Concepts for Distributed HPC Applications

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Gamma Ray Bursts: Science Driver Problem

- Most energetic events known in universe
- Grand challenge in astrophysics; likely to be detected by LIGO in coming years
- Combines many fields of physics
- Requires (at least) petascale computing for modelling
Cactus

- Framework for (tightly coupled) HPC: supports code development, simulation control, analysis, visualisation
- Manage increased complexity with high level abstractions, e.g. for inter-node communication, intra-node parallelisation
- Active user community, 10+ years old
- Supports collaborative development
Cactus in Astrophysics

• Three layers of abstraction in a typical code:
  • *Top*: specific physics codes, developed by single research groups
  • *Middle*: numerical relativity toolkit, developed by community
  • *Bottom*: computational infrastructure, developed by computer scientists
TeraGrid, LONI, LSU, ...

Also: NERSC, Germany, ...

Many machines, all subtly different
Fungible Computing

- Too many machines: need to use them as exchangeable tools, not as unique systems
- TeraGrid Software Stack – excellent idea, but not (yet) successful
- We are building domain-specific abstractions around the HPC machines we use; need to generalise this
BBH Factory: HPC front-end for numerical relativity

- Contains information on: remote access, file system layout, configuring and building, installed software, job submission methods
- Not really domain specific – but application specific and research group specific
- Works great, but is built on simple tools (e.g. ssh), doesn’t scale beyond single group
Fungible Places

• “Places change, people remain the same”

• Cactus supports a truly distributed code development model

• Code components are both developed and stored separately, and are only integrated by the end user

• Numerical relativity groups are “competitive”

single-site research group using many resources

international collaboration
Distributed Code Development

- Mechanism: *ad-hoc interfaces* (Bazaar, no Cathedral)
- Each component describes its interface – there is no abstract base class, *no central authority*
- Only most important interfaces are designed by community

standard object-oriented

"interface"

A

B

type checking when components are activated

A

B

ad-hoc interfaces
What’s Next?

• Above mechanisms are used in production, 24/7 – need to be *reliable*, hence are *boring*

• Other, more exciting Cactus features have been prototyped and demonstrated (see below)

• Not always easy to begin use these in production: need reliability, ubiquity, user buy-in, help desk support
Cactus Framework

- Framework controls execution and manages data
- Components declare what data they access (interface.ccl)
- Components declare which functions they provide (schedule.ccl)
- Components should be functional, i.e., keep no state information
- Thus: Framework has complete state information
- Allows: Checkpointing, correctness checks, metadata collection, and much more...
Multi-Machine Simulations

- LONI: many mid-size machines, fast network: ideal environment to combine compute power

- Using HARC for co-scheduling, Globus for job start and communication

- Can optimise AMR and communication algorithms for heterogeneous networks, since physics and AMR are separated

Using three T3E's in Garching (Germany), Berlin (Germany), and SDSC (USA)
Task Spawning, Job Migration

- As framework, Cactus has complete information about state of the simulation
- Components can query framework, then spawn post-processing jobs, or migrate whole simulation
- Cactus won the High-Performance Computing Challenge Award (SC2002) for a task farming application written with Cactus, which deployed Cactus Black Hole simulations across 70 diverse machines in 12 different countries
Automated Metadata Collection

- Need to preserve metadata about simulations for many reasons, e.g. scientific integrity

- Framework can collect metadata automatically: component *Formaline* saves parameters/events to file, announces them to database

- User does not need to explicitly pass metadata

- Can collect *more data than envisioned by the user*: allows data mining
Remote Visualisation/Steering

Any visualisation client:
Amira, OpenDX, VisIt

Streaming HDF5 auto-downsample

Changing steerable parameters
• Parameters
• Physics, algorithms
• Performance
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CCT: Center for Computation & Technology
Summary

- Cactus has long history of distributed/grid computing; made possible by framework model separating data representation from computations
- Distributed computing is beginning to be production-mode reality for us ("us" = numerical relativity)
- Important: need to stay in control of infrastructure, need to be able to override services
- Problem: not really supported by policies at HPC centres