Enabling Science at the Petascale: From Binary Systems and Stellar Core Collapse to Gamma-Ray Bursts

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Binary neutron star mergers as an engine for short GRBs

- Luminosity $L \sim 10^{48}$ erg s$^{-1}$
- Burst duration $< 2$ s
- Black hole as a result of the merger surrounded by accretion disk generates a jet
- $r$-process nucleosynthesis in the disk and the jet
- Ideal multi-messenger source in neutrinos, gravitational waves, and X-rays

[Etienne et al. 2013]
Core collapse supernovae

- Death of massive stars; explosion energies up to \(10^{53}\text{ erg s}^{-1}\)
- 99% of that energy released in neutrinos
- Explosive nucleosynthesis enriches the interstellar medium with heavy elements
- Typical transient astronomy sources, lightcurves powered by radioactive decay of ejected material

[Ott et al. 2012]
A fraction of type Ic-bl supernovae are observed in combination with a long gamma ray burst/x-ray flash:

What is the engine behind this process and how does it depend on the progenitor parameters? Proto-magnetar or accretion powered collapsar?
Stellar collapse:

- Jet propagation speed, instabilities and asymmetries in the jet geometry
- Tracer particles to track the explosive nucleosynthesis along the outflows of stellar material
- Composition and mass of the ejected material and asymmetries in the ejecta

Neutron star mergers:

- Modeling of merger, accretion phase, black hole and jet formation
- r-process nucleosynthesis in ejected material
Modeling:

- (Ideal) MHD: fluid and magnetic field dynamics
- GR: space-time dynamics, neutron star radius
- Realistic nuclear tabulated EOS: Nuclear interactions
- Neutrino physics and transport: Neutrino interactions (heating, cooling, etc)
- Computational infrastructure: Adaptive mesh-refinement (AMR)
- Multi-D modeling (turbulence, convection, MRI) in massively parallel environments needed!

We use our open-source code GRHydro which is part of the Einstein Toolkit (www.einsteintoolkit.org)!
The **Einstein Toolkit** is

- an open software scientific tool kit for relativistic astrophysics.
- to provide the core computational tools that can enable new science,
- broaden our community,
- facilitate interdisciplinary research,
- take advantage of emerging petascale computers and advanced cyberinfrastructure.

In addition to addressing the **performance** and **scalability** issues, the developers for next generation HPC applications will also need a **sustainable development strategy** to enhance overall programming productivity.
Whenever there is a challenge/difficulty, there is an opportunity. A lot of *multidisciplinary research and analytical work* is involved in

- designing and implementing the right algorithm (applied mathematics, computer science) for the right set of equations (all sciences) on right computing systems (computer science, electrical engineering);
- finding and categorizing the programming patterns (computer science);
- designing and implementing scientific applications (computational sciences);
- and much more...
Our Attempts to Address These Challenges

The prize-winning work at the **SCALE 2009 Challenge** at CCGrid09 is one of our attempts to demonstrate our **multidisciplinary and collaborative research efforts** and **framework-based solutions** to these challenges.
To carry our success to next generation petascale/exascale heterogeneous systems, based on the **Cactus Computational Framework**, we start the **Chemora** project.
Cactus is

- a computational framework for developing portable, modular applications solving partial differential equations.
- focusing, although not exclusively, on high-performance simulation codes.
- designed to allow domain experts in one field to develop modules that are transparent to experts in other fields.
- supporting adaptive mesh refinement via the Carpet library.
- available at http://cactuscode.org/
Carpet is

- a driver layer of Cactus providing adaptive mesh refinement, multi-patch capability, as well as parallelization and efficient I/O.
- written primarily in C++.
- led by Erik Schnetter at LSU and Perimeter Institute.
- available at http://carpetcode.org/
The naive “copy to - compute - copy back” approach in GPU programming very often fails to give optimal performance. As a module (or thorn) in Cactus, we developed an accelerator framework.

- We track which data (and what part of the data) are read and written by a particular routine, and where this routine executes (host or GPU).
- Data are copied only when necessary, and then only those portions that are needed.
- Data are not only accessed for computations; inter-process synchronization and I/O also access data, and are typically executed on the host.
CaKernel Programming Abstractions

CaKernel is

- a kernel abstraction;
- a parallel programming framework suitable for solving some types of PDEs;
- a collection of Cactus modules/thorns;
- able to automatically generate and execute CUDA, OpenCL, and C code;
- the outcome of our collaborative research efforts with PSNC and other institutes.

CaKernel is not

- designed to be a generic solution;
- in its final form yet.
CaKernel contains 3 major parts:

- **CaKernel Descriptor**: is used to declare the variables that will be needed in the computation, and identify a few relevant properties;

- **CaKernel Templates**: are sets of templates which are highly optimized for particular types of computational tasks and optimization strategies;

- **CaKernel Code Generator**: is used to parse the descriptors and automatically generate header files by referring to CaKernel templates. The descriptor parser and code generator are built on Piraha (http://code.google.com/p/piraha-peg/).
Grid Abstractions behind Cactus & CaKernel

- **Grid Hierarchy (GH)** represents the distributed adaptive GH. In Cactus, grid operations are usually handled by a driver thorn to create, operate and destroy hierarchical grid structures.

- **Grid Function (GF)** represents a distributed data structure that represents the variables in an application. The application developers are responsible for providing proper routines to do initialization, boundary updates, etc.

- **Grid Geometry (GG)** represents the coordinates, bounding boxes, and bounding box lists of the computational domain. Operations on the GG, such as union, intersection, refine, and coarsen are usually implemented in a driver thorn as well.
The **CaKernel code generator** parses the CaKernel descriptor and automatically generate CaKernel code from a set of highly optimized templates.
3D Stencil Computation

```c
CCTK_CUDA_KERNEL UPDATE_VELOCITY
TYPE=3DBLOCK
STENCIL="1,1,1,1,1,1"
TILE="16,16,16"
{
  CCTK_CUDA_KERNEL_VARIABLECached=YES \n    INTENT=SEPARATEINOUT
  {
    vx, vy, vz
  } "VELOCITY"
  CCTK_CUDA_KERNEL_VARIABLECached=YES\n    INTENT=IN
  {
    p
  } "PRESSURE"
  CCTK_CUDA_KERNEL_PARAMETER
  {
    density
  } "DENSITY"
}

(credit to P. Micikevicius from NVIDIA)
The Chemora Project

Code Workflow

Cactus variables $U(n)$ are evolved to the next time step $U(n+1)$ during the execution stage.
**Krancc Code Generation Package**

**Krancc** is

- a suite of Mathematica packages with a computer algebra toolbox for numerical relativists.
- a prototyping system for physicists or mathematicians handling very complicated systems of partial differential equations. Krancc can generate entire Cactus based codes starting from a high level set of partial differential equations.
- available at http://krancccode.org/
Kranc is closely coupled with Cactus by

- Defining the grid functions which the simulation will use.
- Performing a user-specified calculation at each point of the grid.
- Computing the right hand sides of evolution equations so that the time integrator can compute the evolved variables at the next time step.
Various kinds of initial value boundary problems:

$$\frac{\partial}{\partial t} u^a = f(u^a),$$
$$u^a|_{t=0} = g(u^a),$$
$$u^a|_{\partial \Sigma} = h(u^a)$$
Mathematical expression:

\[ \partial_t^2 u = \delta^{ab} \partial_b \partial_a u \]

Rewritten in 1st order in time:

\[ \partial_t u = \rho, \]
\[ \partial_t \rho = \delta^{ab} \partial_b \partial_a u \]

Input to Kranc:

\[ \text{dot}[u] \rightarrow \rho, \]
\[ \text{dot}[\rho] \rightarrow KD[ua, ub]PD[u[la], lb] \]
Generated C code to calculate the RHS:

/* Precompute derivatives (new style) */
    PDstandardNth11u = PDstandardNth11(u, i, j, k);
    PDstandardNth22u = PDstandardNth22(u, i, j, k);
    PDstandardNth33u = PDstandardNth33(u, i, j, k);
/* Calculate temporaries and grid functions */
    urhsL = rhoL;
    rhorhsL = PDstandardNth11u + PDstandardNth22u
              + PDstandardNth33u;
/* Copy local copies back to grid functions */
    rhorhs[index] = rhorhsL;
    urhs[index] = urhsL;
The CaKernel parts of Chemora use Kranc-provided and run-time-available information to generate efficient GPU executables from the numerical kernel.

- Stencils and dynamic tile selection (loop tiling, heuristic approaches)
- Lightweight kernel generation (dynamic code generation, index arithmetic simplification)
- Fat kernel detection (loop fusion, code reconstruction, dynamic adjustment of the number of threads)
- Integrated performance monitoring (PAPI, NVIDIA Cupti, kernel identification)
The Chemora Project
Equation Description Language

- Very high level, LaTeX-like syntax for domain scientists
- Description: variables, equations, initial/boundary conditions, parameters, analysis quantities
- A layer between real physics problems to numerical implementations

begin calculation Init
  u = 0
  rho = A \exp(-1/2 \ (r/W)^2)
  v\_i = 0
end calculation

begin calculation RHS
  D\_t u = \rho
  D\_t \rho = \delta^{ij} D\_i v\_j
  D\_t v\_i = D\_i \rho
end calculation

begin calculation Energy
  \epsilon = 1/2 \ (\rho^{\star2} + \delta^{ij} v\_i v\_j)
end calculation
...

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Modeling gravitational waves from binary blackhole system.
The LDC problem describes a initially stationary fluid contained in a square cavity with a moving lid whose velocity is tangent to the lid surface. It is a standard test case for the numerical solvers of the **Incompressible Navier-Stokes equations**.

\[
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla \phi + \nu \nabla^2 \mathbf{u} + \mathbf{f} \tag{1}
\]

\[
\nabla \cdot \mathbf{u} = 0 \tag{2}
\]

where \( \mathbf{u} \) is the velocity field, \( \nu \) is the kinematic viscosity, \( \mathbf{f} \) is the body force, \( \phi \) is the modified pressure (pressure over density).
We solved the LDC problem with a Reynolds number of 100. A comparison of the X component of the velocity field in the midsection along the Y axis with those measured by Ghia et al. (1982) is shown below.
Scaling results of the CFD example on a local cluster.
Conclusions

Targeting Blue Waters and future heterogeneous supercomputers, we designed and implemented Chemora that

- takes a multi-layered approach to enable optimized code for solving complex equations from a high level input,
- is built upon existing computational infrastructures to enable a smooth transition to the next generation computing resources,
- enables synergistic multidisciplinary collaborations,
- could be used in a wide spectrum of scientific applications.
this work was performed using the computational resources of XSEDE, Blue Waters at NCSA, LSU/LONI, and PSNC.