Writing Cactus Thorns

Plan:

- Thorn structure
- HelloWorld thorn
- Solving the Wave Equation
  - standalone code
  - the BadWave thorn
  - advanced thorns: PUGH, MoL, AMR

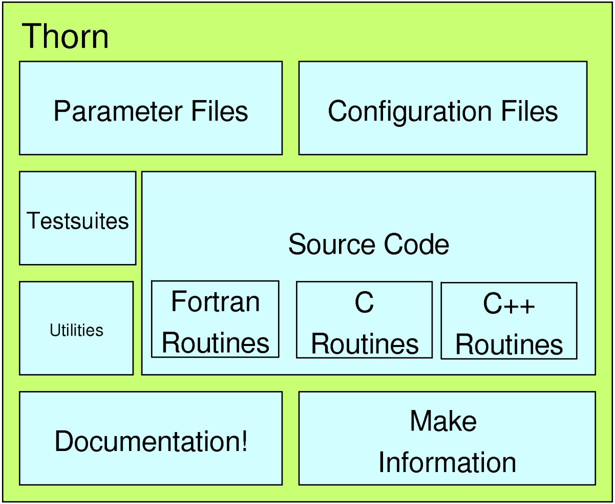
Resources:

- Copy the tutorial files from etk00 home directory:

```
cp -r  /../etk00/tutorial/  /tutorial/
```

Thorn Structure

Inside view of a plug-in module, or thorn for Cactus



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- param.ccl declares:
  - Runtime parameters for the thorn
  - Use/extension of parameters of other thorns

Writing a Hello World thorn

We now demonstrate the process of writing a thorn using a simple Hello World example.

Here is the standalone C code for a Hello World program:

```
#include <stdio.h>
int main(void)
{
  printf("Hello World!\n");
  return 0;
}
```

Creating a New Thorn

To create a stub for a new thorn, type **make newthorn** and follow instructions. A new thorn is created in the **arrangements** directory.

Hello World Thorn

Copy the following into each CCL file:

- `interface.ccl`:

```
implements: HelloWorld
```

- `schedule.ccl`:

```
schedule HelloWorld at CCTK_EVOL
{
  LANG: C
} "Print Hello World message"
```

- `param.ccl`: empty

Hello World Thorn cont.

- src/HelloWorld.c:

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

void HelloWorld(CCTK_ARGUMENTS)
{
  DECLARE_CCTK_ARGUMENTS;
  CCTK_INFO("Hello World!");
  return;
}
```

- make.code.defn:

```
SRCS = HelloWorld.c
```

Running Cactus

- Move to the Cactus/Cactus/par subdirectory
- Create a new file: hello.par
- `hello.par`:

```
ActiveThorns = "HelloWorld"
Cactus::cctk_itlast = 10
```

Running Cactus

- Move to the Cactus/Cactus/thornlists subdirectory
- Create a new file: hello.th
- `hello.th`:

```
Tutorial/HelloWorld
```

Hello World Thorn

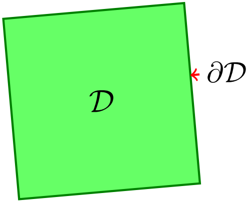
- Screen output:

```
        10
  1   0101       ************************
  01  1010 10      The Cactus Code V4.0
 1010 1101 011      www.cactuscode.org
  1001 100101    ************************
    00010101
     100011     (c) Copyright The Authors
      0100      GNU Licensed. No Warranty
      0101

Cactus version:    4.0.b17
Compile date:      May 06 2009 (13:15:01)
Run date:          May 06 2009 (13:15:54-0500)
[...]

Activating thorn Cactus...Success -> active implementation Cactus
Activation requested for
--->HelloWorld<---
Activating thorn HelloWorld...Success -> active implementation HelloWorld
--------------------------------------------------------------------------------
INFO (HelloWorld): Hello World!
INFO (HelloWorld): Hello World!
[...] 8x
--------------------------------------------------------------------------------
Done.
```

Solving the Wave Equation

The Wave Equation

- PDE which describes wave propagation in a medium
- one of the fundamental equations of mathematical physics
- *For a spatial domain $\mathcal{D}$, find a scalar field $\psi(x, y, z, t)$ which satisfies:*



$$\frac{\partial^2\psi}{\partial t^2} = c^2\nabla^2\psi \qquad \textit{inside } \mathcal{D}\textit{, and}$$

$$B(\psi, \partial_i\psi)|_{\partial\mathcal{D}} = 0 \qquad \textit{at } \partial\mathcal{D}.$$

where c is the speed of the wave,
$B(\psi, \partial_i\psi)$ specifies the boundary conditions,
and ∇^2 is the Laplacian of ψ:

$$\nabla^2\psi \equiv \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]\psi$$

First-order form

The wave equation is a second-order PDE for a single scalar function. To improve its numerical stability properties, we can rewrite it as a system of first-order PDEs:

$$\frac{\partial \psi}{\partial t} = c\vec{\nabla} \cdot \vec{p} \qquad \frac{\partial \vec{p}}{\partial t} = c\nabla\psi$$

with a new unknown vector variable $\vec{p}$. If $\vec{p} = \nabla\psi$, we recover the original scalar wave equation.

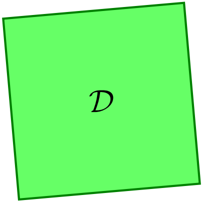
We are going to solve this system of PDEs inside a *cube* $\mathcal{D} = [-a, a]^3$ with the following boundary conditions:

$$\psi|_{\partial\mathcal{D}} = 0 \qquad \vec{p}_{\|}|_{\partial\mathcal{D}} = 0 \qquad \vec{p}_{\perp}|_{\partial\mathcal{D}_{i+}} = \vec{p}_{\perp}|_{\partial\mathcal{D}_{i-}}$$

where $\vec{p}_{\perp}$, $\vec{p}_{\|}$ are the (outward) normal and tangential components of $\vec{p}$, and $\partial\mathcal{D}_{i+}/\partial\mathcal{D}_{i-}$ are the opposite faces normal to the i-th axis.

Discretization

We will be solving the wave equation using finite difference (FD) methods on rectangular grids (adding mesh refinement later).



- spatial domain $\rightarrow$ rectangular grid
- continuous function $\rightarrow$ grid function
- partial derivative $\rightarrow$ FD operator
- PDE $\rightarrow$ system of algebraic equations

$$\left.\begin{array}{l} \frac{\partial\psi}{\partial t} = c\vec{\nabla}\cdot\vec{p} \\[2em] \frac{\partial\vec{p}}{\partial t} = c\nabla\psi \end{array}\right| \rightarrow \left| \begin{array}{l} D_t\psi = K_\psi := c(D_x p_x + D_y p_y + D_z p_z) \\ D_t p_x = K_x := cD_x\psi \\ D_t p_y = K_y := cD_y\psi \\ D_t p_z = K_z := cD_z\psi \end{array}\right.$$

where D_t, D_x, D_y and D_z are the *finite differencing* operators.

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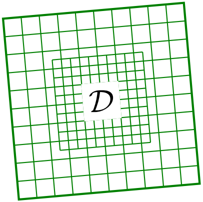

- spatial domain → rectangular grid
- continuous function → grid function
- partial derivative → FD operator
- PDE → system of algebraic equations

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where D_t, D_x, D_y and D_z are the *finite differencing* operators.

Spatial derivatives

We approximate spatial derivatives by finite differences of the grid function values at neighboring points. We will use a centered scheme, which is second-order accurate in grid spacing Δ:

$$(D_x\psi)_{i,j,k} = \frac{\psi_{i+1,j,k} - \psi_{i-1,j,k}}{2\Delta}$$

$$(D_y\psi)_{i,j,k} = \frac{\psi_{i,j+1,k} - \psi_{i,j-1,k}}{2\Delta}$$

$$(D_z\psi)_{i,j,k} = \frac{\psi_{i,j,k+1} - \psi_{i,j,k-1}}{2\Delta}$$

Runge-Kutta time integration

Simplest Runge-Kutta method: Neuton integration (1st order accurate)

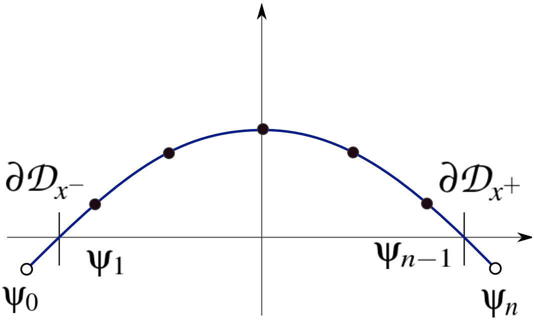
$$\frac{y_{n+1} - y_n}{\Delta t} = K_y(t_n, y_n) \qquad \rightarrow \qquad y_{n+1} = y_n + K_y(t_n, y_n)\Delta t$$

We will use a 2nd order accurate Runge-Kutta integration scheme (also known as a *Heun method*) with two intermediate steps:

$$\begin{aligned} k_1 &= K_y(t_n, y_n) \\ \tilde{y}_n &= y_n + k_1 \Delta t, \\ k_2 &= K_y(t_n + \Delta t, \tilde{y}_n) \\ y_{n+1} &= y_n + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)\Delta t \end{aligned}$$

Discrete boundary conditions

We place the grid points in such a way that the boundary of the domain $\partial\mathcal{D}$ lies in between the two last grid points:

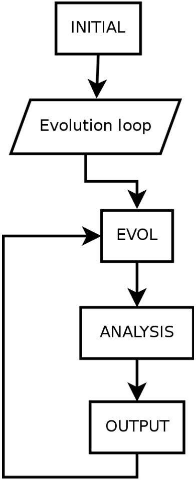


$$\psi|_{\partial\mathcal{D}} = 0$$
$$\vec{p}_{\parallel}|_{\partial\mathcal{D}} = 0$$
$$\vec{p}_{\perp}|_{\partial\mathcal{D}_{i+}} = \vec{p}_{\perp}|_{\partial\mathcal{D}_{i-}}$$
$$\Downarrow$$
$$\psi_{0,j,k} = -\psi_{1,j,k},$$
$$\vec{p}_{y,0,j,k} = -\vec{p}_{y,1,j,k},$$
$$\vec{p}_{z,0,j,k} = -\vec{p}_{z,1,j,k},$$
$$\vec{p}_{x,0,j,k} = \vec{p}_{x,1,j,k},$$

... *etc.*

Standalone code

```
int main(int argc,char **argv) {
    FILE *fp = fopen("psi.d.asc","w+");
    BadWave_Init();
    BadWave_ApplyBounds();
    BadWave_print(fp);
    // evolve 100 steps
    for(int i=0;i<100;i++) {
        iter = i;
        BadWave_Evolve();
        BadWave_ApplyBounds();
        BadWave_Evolve2();
        BadWave_TmpApplyBounds();
        BadWave_print(fp);
    }
    fclose(fp);
    return 0;
}
```



Standalone code: parameters and definitions

```
// Parameters:
bool verbose = true;      // enable verbose output
double wave_speed = 1.0; // wave speed factor
const int isiz = 32, jsiz = 32, ksiz = 32; //grid size

// 1D array to hold the grid and a function to find 3D indices
typedef double gridfunc[isiz*jsiz*ksiz];
inline int INDEX3D(int i,int j,int k) { return (i+j*isiz)*ksiz+k; }

// Grid functions:
gridfunc psi,px,py,pz;              // psi and p
gridfunc tpsi,tpx,tpy,tpz;          // temporary variables
gridfunc kpsi,kpx,kpy,kpz;          // the kernels
gridfunc k2psi,k2px,k2py,k2pz;

// Other global variables: iteration, grid spacing and time step
int iter=0;    double dx, dy, dz, dt;
```

Writing thorn BadWave: param.ccl

```
# Parameter definitions for thorn BadWave

private:
CCTK_REAL wave_speed "characteristic speed at boundary"
{
  "0.1:*" :: "wave speed"
} 1.

private:
CCTK_BOOLEAN verbose "whether to print stuff"
{
    :: "verbose flag"
} 0
```

Writing thorn BadWave: interface.ccl

```
# Interface definition for thorn BadWave
implements: BadWaveTutorial
inherits: grid

CCTK_REAL wave_vars TYPE=gf
{
    psi
    px, py, pz
} "Basic components of wave equation code"

CCTK_REAL tmp_wave_vars TYPE=gf { tpsi, tpx, tpy, tpz } <...>
CCTK_REAL kernels TYPE=gf {
    kpsi kpx, kpy, kpz, k2psi, k2px, k2py, k2pz
} <...>
```

Writing thorn BadWave: schedule.ccl

```
# Schedule definitions for thorn BadWave
storage: wave_vars, tmp_wave_vars, kernels

schedule BadWave_Init at INITIAL
{ LANG: C
} "Startup and initialize"

schedule BadWave_ApplyBounds at POSTSTEP
{   LANG: C
    SYNC: wave_vars
} "Apply boundary conditions"

schedule BadWave_Evolve at EVOL <...>
schedule BadWave_TmpApplyBounds at EVOL after BadWave_Evolve <...>
schedule BadWave_Evolve2 at EVOL after BadWave_TmpApplyBounds <...>
```

Adapting the source code for Cactus

Modifications to standalone code:

- include Cactus headers:

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

- declare all scheduled functions with external C linkage:

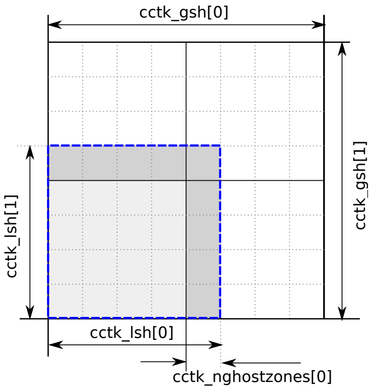
```
extern "C" void BadWave_Init(CCTK_ARGUMENTS);
extern "C" void BadWave_ApplyBounds(CCTK_ARGUMENTS);
extern "C" void BadWave_TmpApplyBounds(CCTK_ARGUMENTS);
extern "C" void BadWave_Evolve(CCTK_ARGUMENTS);
extern "C" void BadWave_Evolve2(CCTK_ARGUMENTS);
```

- add the CCTK_ARGUMENTS macro to scheduled functions:

```
void BadWave_Init(CCTK_ARGUMENTS)
{
    DECLARE_CCTK_ARGUMENTS;
    ...
}
```

this tells functions which part of the grid they will be working on.

Grid definitions in Cactus



- cctk_gsh: global grid dimensions
- cctk_lsh: local grid dimensions
- cctk_delta_space: grid spacing
- cctk_nghostzones: number of ghostzones
- cctk_bbox: whether a boundary is an outer one
- CCTK_GFINDEX3D(i,j,k): computes local 1D grid index

Simple parameter file

Parfile: `par/BadWavePUGH.par`

- include the driver thorn (PUGH)
- specify grid size
- specify BadWave parameters

```
ActiveThorns = "BadWave PUGH"

cactus::cctk_itlast   = 100
pugh::global_nsize    = 32
pugh::ghost_size      = 1

BadWavePUGH::wave_speed = 2.0
```

More advanced parameter file

Parfile: `par/BadWavePUGHv2.par`

Includes new thorns:

- `CoordBase`: coordinate extents
- `CardGrid3D`: provides variety of grid configurations
- `SymBase`: basic thorn for specifying symmetries of the domain
- `IOBasic`, `IOUtil`, `IOScalar`, `IOASCII`: basic and advanced I/O
- `Time`: provides global time and iteration variables
- `PUGHSlab`, `PUGHReduce`, `LocalReduce`: required by I/O thorns

Method of Lines

- Method of lines is a general name for an approach of solving PDEs with time variable, in which the PDE is approximated by a system of interdependent ODEs for each grid point.
- Method of lines allows to extend time integration methods developed for ODEs to PDEs.
- Cactus thorn MoL implements several different time integration methods.
- We can use these methods if we modify our thorn: `BadWaveMoL`

Registering evolved variables with MoL

- in Wave.cc:

```
void BadWaveMoL_Register(CCTK_ARGUMENTS)
{
    DECLARE_CCTK_ARGUMENTS;
    MoLRegisterEvolved(CCTK_VarIndex("BadWaveMoL::psi"),
                       CCTK_VarIndex("BadWaveMoL::kpsi"));
    ...
}
```

- in schedule.ccl:

```
storage: wave_vars[3], kernels[3]
schedule BadWaveMoL_Register in MoL_Register
{
    LANG: C
} "Register for MoL"
```

Registering evolved variables with MoL

- in `interface.ccl`:

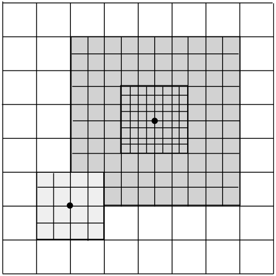
```
CCTK_INT FUNCTION MoLRegisterEvolved \
  (CCTK_INT IN EvolvedIndex, CCTK_INT IN RHSIndex)
USES FUNCTION MoLRegisterEvolved
```

- in the parfile (`par/BadWaveMoL.par`):

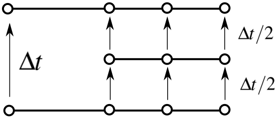
```
ActiveThorns = "BadWaveMoL carpet
CarpetIOBasic CarpetIOASCII CarpetIOScalar CarpetLib LoopC
IOUtil SymBase Time CarpetReduce CartGrid3D MoL"

MoL::ODE_Method = "RK4"
MoL::MoL_Intermediate_Steps = 4
MoL::MoL_Num_Scratch_Levels = 1
```

Berger-Oliger mesh refinement

- "Box-in-box" refinement:



- Time update:



- STARTUP
  PARAMCHECK
- BASEGRID
  ↑ INITIAL, POSTINITIAL
- ↓ RESTRICT
- ↑ ANALYSIS
- Main loop
  - ↑ REGRID
  - ↑ Advance time
    EVOL (incl. MoL)
  - ↓ RESTRICT
  - ↑ CHECKPOINT
    ANALYSIS

Fixed mesh refinement

Parfile: par/BadWaveFMR.par

```
ActiveThorns = "CarpetRegrid2 Dissipation
SpaceMask SphericalSurface"

CarpetRegrid2::num_levels_1 = 2
Carpet::max_refinement_levels = 2
CarpetRegrid2::num_centres = 1
CarpetRegrid2::Position_x_1 = 0.5
CarpetRegrid2::Position_y_1 = 0.5
CarpetRegrid2::Position_z_1 = 0.5
CarpetRegrid2::radius_1[1] = 0.1
#CarpetRegrid2::radius_1[2] = 0.1
CarpetRegrid2::verbose = "yes"
Carpet::init_fill_timelevels="yes"
Dissipation::vars = "BadWaveMoL::psi"
```

Adaptive mesh refinement

Modifications to the code:

```
void BadWaveAMR_BoxMover(CCTK_ARGUMENTS)
{
    DECLARE_CCTK_ARGUMENTS;
    int max_refinement_levels = 30;

    radius[max_refinement_levels*0+1]=.05;

    // Make the box wiggle
    position_x[0] = position_y[0] = position_z[0] = 0.7+0.05*sin(cctk_time)
    active[0]=1;
    num_levels[0]=2; // two levels: 0=base grid, 1=first refined grid

    // Turn on the next box
    active[1] = 1;
    radius[max_refinement_levels*1+1]=.05;
    position_x[1]=position_y[1]=position_z[1]=.3;
    num_levels[1]=2;
}
```

Adaptive mesh refinement

- Modifications to the `schedule.ccl`:

```
schedule BadWaveAMR_BoxMover at preregrid
{
    LANG: C
} "Jiggle the box"
```

- Modifications to the `interface.ccl`:

```
inherits: grid, CarpetRegrid2
```

Adaptive mesh refinement

Modifications in the parfile (pars/BadWaveAMR.par):

```
CarpetRegrid2::regrid_every = 2
Carpet::max_refinement_levels = 3
CarpetRegrid2::num_centres = 2

CarpetRegrid2::num_levels_1 = 3
CarpetRegrid2::Position_x_1 = 0.3
CarpetRegrid2::Position_y_1 = 0.3
CarpetRegrid2::Position_z_1 = 0.3
CarpetRegrid2::radius_1[1] = 0.2
CarpetRegrid2::radius_1[2] = 0.1

CarpetRegrid2::num_levels_2 = 2
CarpetRegrid2::Position_x_2 = 0.7
CarpetRegrid2::Position_y_2 = 0.7
CarpetRegrid2::Position_z_2 = 0.7
CarpetRegrid2::radius_2[1] = 0.05
```

Adaptive mesh refinement

Modifications in the parfile (pars/BadWaveAMR.par):

```
ActiveThorns = "IOJPeg CarpetSlab CarpetInterp
         CarpetInterp2 AEILocalInterp"
IOJpeg::out_every                = 1
IOJpeg::out_vars                 = "BadWaveAMR::psi"

IOJPeg::gridpoints = interpolate
IOJpeg::array2d_x0          = 0.0
IOJpeg::array2d_y0          = 0.0
IOJpeg::array2d_z0          =  0.5
IOJpeg::array2d_npoints_i   = 101
IOJpeg::array2d_dx_i        =  0.01
IOJpeg::array2d_dy_i        =  0
IOJpeg::array2d_dz_i        =  0
IOJpeg::array2d_npoints_j   = 101
IOJpeg::array2d_dx_j        =  0
IOJpeg::array2d_dy_j        =  0.01
IOJpeg::array2d_dz_j        =  0
```