Requirements for a new EOS interface in the Einstein Toolkit

Erik Schnetter, 2009-11-03
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Discussion Topic

• Topic: Requirements for a new EOS interface

• Background: Plan to restructure current EOS interface (EOSBase) for future needs

• Today: Collect / brainstorm requirements

• Will then discuss design and implementation by email
Cactus EOS Interface

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XiRel phone call, 3 November 2009
Outline

1 Requirements

2 Interfaces
   - Original interface
   - “New” interface

3 Wishlist
An EOS logically closes the system of equations. Specifically, given some set of *independent* thermodynamic potentials (some subset of $\rho$, $\varepsilon$, composition, entropy, temperature, . . .) all remaining *dependent* quantities (pressure, speed of sound, entropy, . . .) are given by the EOS.

The EOS must specify
- which independent variables it requires;
- which dependent variables it can compute.
In CactusEOS there exists the original EOS_Base interface.

- Assumes that independent variables are exactly two of $\rho, \varepsilon, P$.
- Only potential dependent variables are $\rho, \varepsilon, P, P_\rho, P_\varepsilon$.
- Uses direct function pointers (pre-function aliasing).
- Calls not set up in advance - no need.
- All calls are pointwise.
- Function prototypes fully specified - e.g.
  \[
  \text{press}(i,j,k) = \text{EOS\_Pressure}(\text{handle}, \ \rho(i,j,k), \ \varepsilon(i,j,k)).
  \]
"New" interface

In Whisky_Dev a new interface EOSBase_General exists but is little used.

- (In)dependent variable numbers and names arbitrary.
- Uses function aliasing.
- Works on whole grid functions (∃ array interface, can be used for pointwise calls - overly complex).
- Calls set up in advance and cached using tables.
- Function prototypes specified, but order of (in)dependent variables not - e.g.

```c
ierr = EOS_SetGFs(cctkGH, EOS_Con2PrimCall).
```

Here `EOS_Con2PrimCall` is a table handle.
Wishlist

EOS interface must be able to
- deal with arbitrary (in)dependent variables.
- work pointwise or with grid functions, and do it efficiently.
- be simple for simple cases.
- extend to table readers with fallback mechanisms.

EOS interface should be able to
- deal with masks (excision, atmosphere) when using GFs.
- deal with multiple, possibly dynamically changing EOSs.
- provide a fallback mechanism for local failures.
EOS interface

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October 30, 2009
EOS calls in Whisky

- Con2Prim: pointwise only; iterative
- Prim2Con: mostly for the whole grid, pointwise in AtmosphereReset
- Eigenproblem in Riemann solvers (Roe, Marquina): acts on whole grid
- (modified) PPM reconstruction: only pointwise interface used
Current EOS shortcomings

old interface
- hard-coded dependent and independent variables
- EOSBase.h needs to be included in header of each (Fortran) function that uses EOS routines
- Cactus is not aware of the functions provided (not aliased)
- possible function call overhead at each point if whole grid function is processed (this should be small however)

new (general) interface
- setup of calls is too complicated and error prone
- not publicly available (?)
HydroBase: record EOS associated with primitives
EOS interface should be simple to use
keep number of temporary grid functions to a minimum
maybe detect common errors at compile time (i.e. misspelled variable names)
fallback/alternative EOS mechanism (for Con2Prim)