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Title: Equation of State Interface for Hydro Applications

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Equation of State Interface for Hydro Applications

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A key input for hydro simulations is an equation of state. An interface, in conjunction with an equation of state library, is needed in order for different codes to access the same material models and a user to specify materials in a uniform manner. In addition the design of an interface should take account of ease of use and convenience, such as a syntax that strives to minimize the occurrence of common input errors and to facilitate validation tests. The requirements of an EOS package and a software design to meet these needs are presented. The design has been implemented in the Amrita environment and demonstrated on test problems. A similar approach would be of value for other hydro components.

Equation of State Interface for Hydro Applications

Ralph Menikoff, T-14

&

James J. Quirk, CCS-2

January, 2003

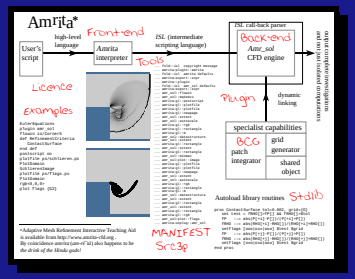
Requirements for EOS package

- Capabilities – thermodynamics
  - Evaluate thermodynamic quantities
  - Hydro routines
  - Treat all EOS in uniform manner
- Extendable – long lived
  - Add new materials
  - Composite models
  - Additional constitutive properties
- Ease of Use – preferred method
  - Common interface
  - Example script
  - Specify material by name
  - Validation of EOS
- Convenience – less error prone
  - Conversion of units
  - Infer (V, e, u) from other data
  - User friendly

Software design

- EOS package
  - Database for parameters
  - Application interface & library
  - Shared objects for implementing models
  - Auxiliary routines

- Amrita
  (James Quirk)



  - Interpreter/Parser, **front end**
  - Computational engine, **back end**
  - Keywords for specialized applications
  - Read & write channels between front and back ends

- Coupling EOS with hydro algorithm
  - Euler equations with multi-materials
  - Patch integrator for *amrsol*
  - EOS plugin for Amrita

Amrita script for Hydro application

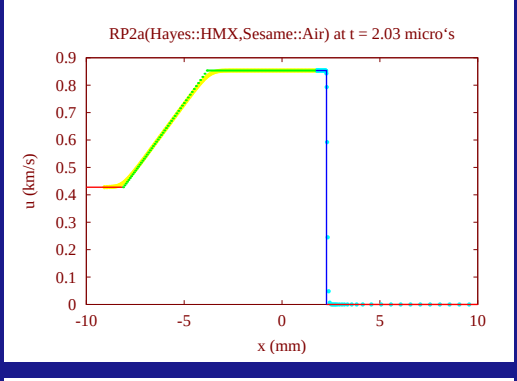
General structure of script

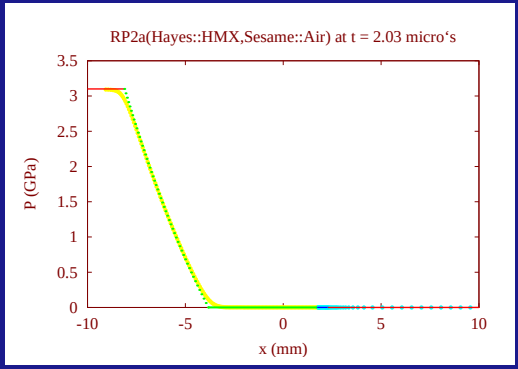
- Initialize resources
- Set input parameters
- Prescribe problem
- Run simulation/Generate data
- Post-process/Typeset results

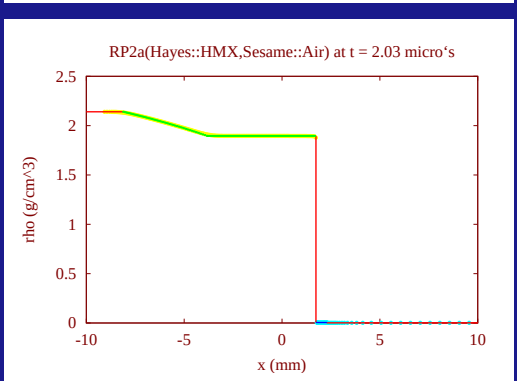
Example simulation

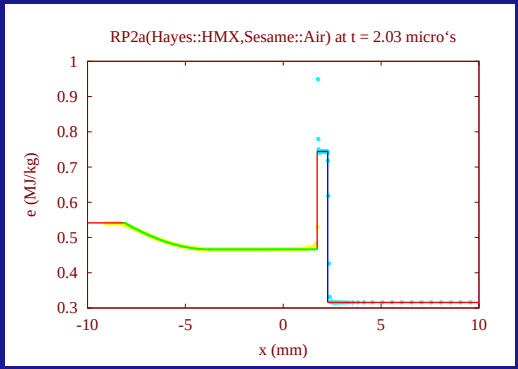
Riemann problem with two different materials

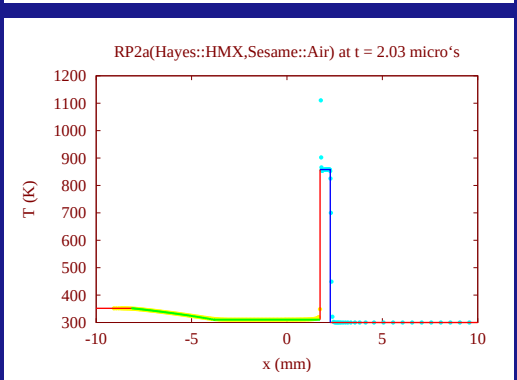
Example Results

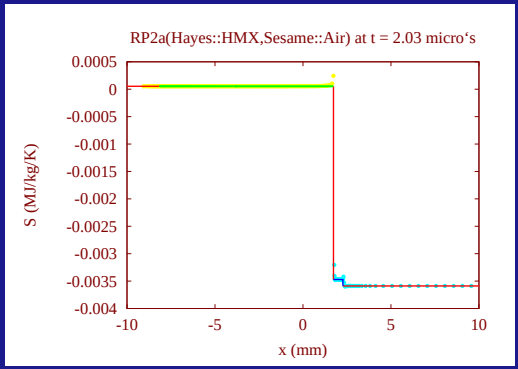












Entropy error at interface

Summary of Approach

- Identify common patterns of work
  Idiomatic/Ease of Use
- Specialized scripting language
  Automation/Reliability/Validation
- Dynamically linked libraries
  Extendable system/Flexible