ExactPack: An Open-Source Software Package for Code Verification

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ExactPack: An Open-Source Software Package for Code Verification

- Test problem analytic and semi-analytic solvers
- Code verification analysis tools
- Designed to enable adding new solvers and analysis tools

ExactPack is available for download and collaboration at

www.github.com/losalamos/exactpack

We would like to see this tool be used and contributed to by the wider V&V community!
ExactPack: An Open-Source Software Package for Code Verification

• Role of ExactPack in the verification Process
• Verification test problem solvers in ExactPack
• Verification analysis capabilities in ExactPack
• ExactPack use cases & documentation
• Software demonstration of ExactPack
ExactPack plays a specific role in our overall code and solution verification infrastructure

Verification Test Suite

Standardized problem definitions

Code input files

Report templates

Computational Physics Codes

ExactPack

Reference solutions

Verification analysis tools

Driver Package
ExactPack contains solvers for many common computational physics verification test problems

- **Hydrodynamics**
  - Noh, Sedov, Guderley
  - Several common Riemann shock tube problems (Sod, Einfeldt, Stationary Contact, Slow Shock, Shock Contact Shock, LeBlanc)
  - Shock tube problem with JWL equation of state
- **Reactive flows**
  - Escape of high-explosive products
  - Kenamond programmed burn timing
  - Steady-detonation reaction zone
  - Mader
- **Inviscid hydrodynamics with heat transfer (radiation, conduction)**
  - Coggeshall
  - Reinicke Meyer-ter-Vehn
  - Su-Olson
- **Solid mechanics**
  - Blake
Several new solvers are under development in ExactPack

- **Hydrodynamics**
  - Noh’s uniform collapse problem
- **Reactive flows**
  - Detonation Shock Dynamics (DSD) test problems
  - Steady Zel’dovich-von Neumann-Döring (ZND) wave tests for arbitrary reaction rate law and equation of state
- **Inviscid hydrodynamics with heat transfer (radiation, conduction)**
  - Lowrie-Rauenzahn equilibrium diffusion
  - Lowrie-Edwards non-equilibrium diffusion
  - Plasma diffusion
- **Solid mechanics**
  - Tests of flow stress and friction models
ExactPack provides tools for code verification analysis

• Load data from computational physics code results
• Call exact solution from ExactPack solvers at grid points of interest
• Compute error norms using values of physical variables in computational and exact solutions
• Compute convergence rates of error norms
• Display results in a standardized format

Caution: This part of the code package is still very much under active development
ExactPack use case: Generate and plot analytic solutions

from exactpack.solvers.riemann import Sod

r = numpy.linspace(0.0, 1.0, 1000)
t = 0.25

solver = Sod()
soln = solver(r, t)

soln.plot('density')
soln.plot('pressure')
soln.plot('velocity')

In-line in a hydrodynamics code:
• Import solver object
• Instantiate solver object once
• Evaluate solver at vector of grid points at each desired time step
ExactPack use case: Code verification study

```python
from exactpack.sedov.riemann import Sod
from exactpack.analysis import CodeVerificationStudy

study = CodeVerificationStudy(code_output, Sod(pl=1e5, pr=1e4, interface_loc=0.0), d(xs=[0.02, 0.01, 0.005], domain=(0, 1.0), time=0.007, reader=code_reader)

study.plot('velocity_x')

study.convergence('velocity_x', norm=PointNorm().plot(fiducial=2./3.)
```

![Graph of velocity_x vs position](image1.png)

![Graph of L1 error norm vs initial zone size](image2.png)
ExactPack is thoroughly documented

ExactPack is a collection of exact hydrodynamics solutions packaged as an easy to use Python library with a uniform interface. In this context, an exact solution is not necessarily an analytic expression. Most solutions provided by the library actually require the solution of an ordinary differential equation or the numerical approximation of an integral.

The primary purpose of ExactPack is to provide reference solutions for validation and command-line utility are both also provided, which makes it easy to use.

- 1. Quickstart Guide
  - 1.1. Installation
  - 1.2. The ExactPack Graphical User Interface
  - 1.3. Using ExactPack from the Command Line
  - 1.4. Using ExactPack as a Python Library
- 2. User’s Guide
  - 2.1. Available Solvers
  - 2.2. The Solver Class
- 3. Developer’s Guide
  - 3.1. Coding Style
  - 3.2. A Tour of the Package Source
  - 3.3. Adding a New Solver
- 4. Reference Guide
  - 4.1. Core Functionality
  - 4.2. Interfaces
- 5. Solvers
  - 5.1. Coggeshall Problem
  - 5.2. The Escape of HE Products Problem
  - 5.3. The Mader Problem
  - 5.4. The Noh Problem
  - 5.5. The Riemann Solver
  - 5.6. The Richtmeyer-Meshkov-Venkada Problem
  - 5.7. The Sedov Problem
  - 5.8. The Su-Olson Problem
- 6. Testing
  - 6.1. The Escape of HE Products Problem
  - 6.2. The Mader Problem
  - 6.3. The Noh Problem
  - 6.4. The Riemann Problem
  - 6.5. The Richtmeyer-Meshkov-Venkada Problem
  - 6.6. The Sedov Problem
  - 6.7. The Su-Olson Problem

5.5. The Riemann Solver
The independent fluid variables are (i) the gas density $\rho(r, t)$, (ii) the velocity of the gas $u(r, t)$, and (iii) the pressure $P(r, t)$, each at spatial location $r$ and time $t$. The specific internal energy $e(r, t)$ is related to the other fluid variables by the equation of state (EOS) for an ideal gas at constant entropy, $P = (\gamma - 1)\rho e$,

where $\gamma = c_p/c_v$ is the ratio of specific heats at constant pressure and volume. For a mono-atomic ideal gas we have $\gamma = 5/3$. The Euler equations take the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0$$

$$\frac{\partial e}{\partial t} + \frac{\partial (ue)}{\partial x} = -\rho \frac{\partial P}{\partial x}$$

where $x = 1, 2, 3$ for planar, cylindrical, and spherical coordinates respectively.

The gas starts out with constant values of density, velocity, and pressure in two contiguous regions delimited by a distance $n_0$.

$$r < n_0 : \begin{align*}
\rho(r, 0) &= \rho_1 \\
\rho(r, 0) &= \rho_2 \\
\rho(r, 0) &= P_1 \\
\rho(r, 0) &= P_2 .
\end{align*}$$

The documentation uses the Sphinx toolbox and can be generated in HTML, LaTeX, or PDF format.
Near-term plans for ExactPack development

• Exercise ExactPack for code verification using contents of LANL Verification Test Suite
• Refactor ExactPack for data structure from VTK Visualization Toolkit to facilitate better use of mesh-based data
• Implement new optimization-based method for code convergence analysis
• Implement additional test problems mentioned previously
Longer-term plans for ExactPack development

- Solution Verification
- Method of Manufactured Solutions
- Method of Nearby Problems
- In conjunction with Verification Test Suite:
  - Standardized problem and implementation definitions
  - Semi-automated verification problem setup, execution, and analysis