The Riemann Problem and General Equations of State

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Equations of State

An equation of state (EOS) is a set of equations relating state parameters (e.g. density, pressure, energy) of a fluid.

$\rho =$ Density

$u =$ 1D Velocity

$p =$ Pressure

$s =$ Specific entropy

$E =$ Total energy density

$\epsilon =$ Specific internal energy

$H =$ Specific enthalpy

$a =$ Adiabatic sound speed

Ideal EOS

$$p = (\gamma - 1)\rho\epsilon$$

$$E = \frac{1}{2}\rho u^2 + \frac{p}{\gamma - 1}$$

$$H = \frac{1}{2}u^2 + \left(\frac{\gamma}{\gamma - 1}\right)\frac{p}{\rho}$$

$$a^2 = \gamma\frac{p}{\rho}$$

General EOS

$$p = p(\rho, \epsilon) \text{ or } \epsilon = \epsilon(\rho, p)$$

$$E = \frac{1}{2}\rho u^2 + \rho\epsilon$$

$$H = \frac{1}{2}u^2 + \epsilon + \frac{p}{\rho}$$

$$a^2 = \left(\frac{\partial p}{\partial \rho}\right)_s$$

Assumptions: $\dfrac{\partial p}{\partial \rho} > 0, \quad \dfrac{\partial p}{\partial \epsilon} > 0$

The Riemann Problem

Simple 1D hydrodynamics problem

ρ = Density

u = Velocity

p = Pressure

E = Energy density

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \text{ (mass cons.)}$$

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0 \text{ (mom. cons.)}$$

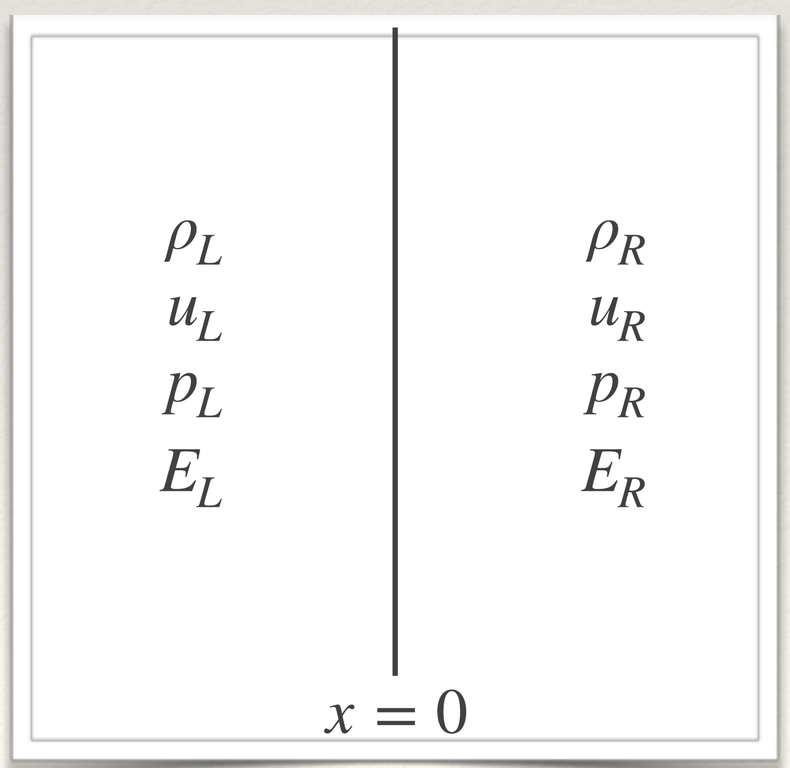
$$\frac{\partial E}{\partial t} + \frac{\partial (E + p)u}{\partial x} = 0 \text{ (energy cons.)}$$

$$E \equiv \frac{\rho u^2}{2} + \rho\epsilon$$

$\epsilon = \epsilon(\rho, p)$ or

$p = p(\rho, \epsilon)$

Initial Conditions



Find

$\rho(x,t)$, $u(x,t)$, $p(x,t)$, $E(x,t)$ for $x \in \mathbb{R}$, $t \geq 0$

The Riemann Problem

Vector form (quasilinear approximation)

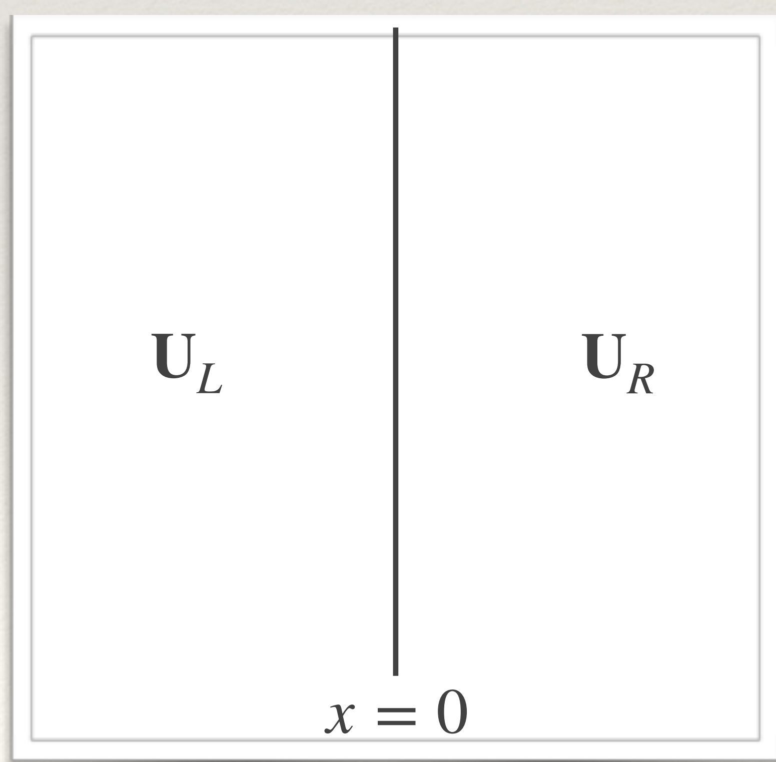
$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} \qquad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u \rho H \end{pmatrix} = \begin{pmatrix} U_2 \\ U_2^2 / U_1 + p(\mathbf{U}) \\ U_2 / U_1 (U_3 + p(\mathbf{U})) \end{pmatrix}$$

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}\left(\mathbf{U}\right)}{\partial x} = 0$$

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}\left(\mathbf{U}\right) \frac{\partial \mathbf{U}^{\mathrm{T}}}{\partial x} = 0$$

$$H \equiv \frac{1}{2} u^2 + \epsilon + \frac{p}{\rho}$$

Initial Conditions



Evaluate and simplify A

$$\mathbf{A}(\mathbf{U}) \equiv \frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \begin{pmatrix} 0 & 1 & 0 \\ p_1 - \left(\frac{U_2}{U_1}\right)^2 & p_2 + \frac{2U_2}{U_1} & p_3 \\ \frac{U_2 p_1}{U_1} - \frac{U_2 (p + U_3)}{U_1^2} & \frac{p + U_3}{U_1} + \frac{p_2 U_2}{U_1} & \frac{U_2 (p_3 + 1)}{U_1} \end{pmatrix}$$

$$p_i(\rho, \epsilon) \equiv \frac{\partial p}{\partial U_i} = p_\rho \frac{\partial \rho}{\partial U_i} + p_\epsilon \frac{\partial \epsilon}{\partial U_i}$$

$$p_\rho \equiv \partial p / \partial \rho$$

$$p_\epsilon \equiv \partial p / \partial \epsilon$$

The Riemann Problem

After lots of math and the 2nd law of thermodynamics

$$\mathbf{A}(\mathbf{U}) = \begin{pmatrix} 0 & 1 & 0 \\ a^2 + \frac{(u^2 - H)p_\epsilon}{\rho} - u^2 & u\left(2 - \frac{p_\epsilon}{\rho}\right) & \frac{p_\epsilon}{\rho} \\ \frac{u\left(a^2\rho - H(p_\epsilon + \rho) + u^2 p_\epsilon\right)}{\rho} & H - \frac{u^2 p_\epsilon}{\rho} & \frac{u(p_\epsilon + \rho)}{\rho} \end{pmatrix}$$

$$\overbrace{a^2 \equiv \left(\frac{\partial p}{\partial \rho}\right)_s}^{\text{Adiabatic sound speed}} = \overbrace{\frac{p}{\rho^2} p_\epsilon + p_\rho}^{\text{Uses 2nd law}}$$

$$= \frac{1}{\epsilon_p}\left(\frac{p}{\rho^2} - \epsilon_\rho\right)$$

Eigenvalues/ wave speeds	Left eigenvectors	Right eigenvectors
$\lambda_1 = u - a$	$\mathbf{l}^{(1)} = \left(\frac{p_\epsilon}{\rho}(H - u^2) - a(a+u),\ u\frac{p_\epsilon}{\rho} + a,\ -\frac{p_\epsilon}{\rho}\right)$	$\mathbf{r}^{(1)} = \begin{pmatrix} 1 \\ u - a \\ H - au \end{pmatrix}$
$\lambda_2 = u$	$\mathbf{l}^{(2)} = \left(H - u^2,\ u,\ -1\right)$	$\mathbf{r}^{(2)} = \begin{pmatrix} 1 \\ u \\ H - \frac{a^2\rho}{p_\epsilon} \end{pmatrix}$
$\lambda_3 = u + a$	$\mathbf{l}^{(3)} = \left(\frac{p_\epsilon}{\rho}(H - u^2) - a(a-u),\ u\frac{p_\epsilon}{\rho} - a,\ -\frac{p_\epsilon}{\rho}\right)$	$\mathbf{r}^{(3)} = \begin{pmatrix} 1 \\ u + a \\ H + au \end{pmatrix}$

The Riemann Problem

Three types of waves

Rarefaction/simple wave

$\mathbf{l}^{(i)} \cdot \mathrm{d}\mathbf{U} = 0$

Reduces to $\mathrm{d}s = 0,\ \ \mathrm{d}u = \pm\, a \dfrac{\mathrm{d}\rho}{\rho}$

Contact wave/discontinuity

$\dfrac{\mathrm{d}U_i}{\mathbf{r}_i^{(2)}} = \dfrac{\mathrm{d}U_j}{\mathbf{r}_j^{(2)}}$ for all $i, j \in \{1,2,3\}$

Reduces to $\mathrm{d}p = 0,\ \ \mathrm{d}u = 0$

Shock wave (non-linear)

Fluxes are conserved across shock:
Rankine-Hugoniot conditions

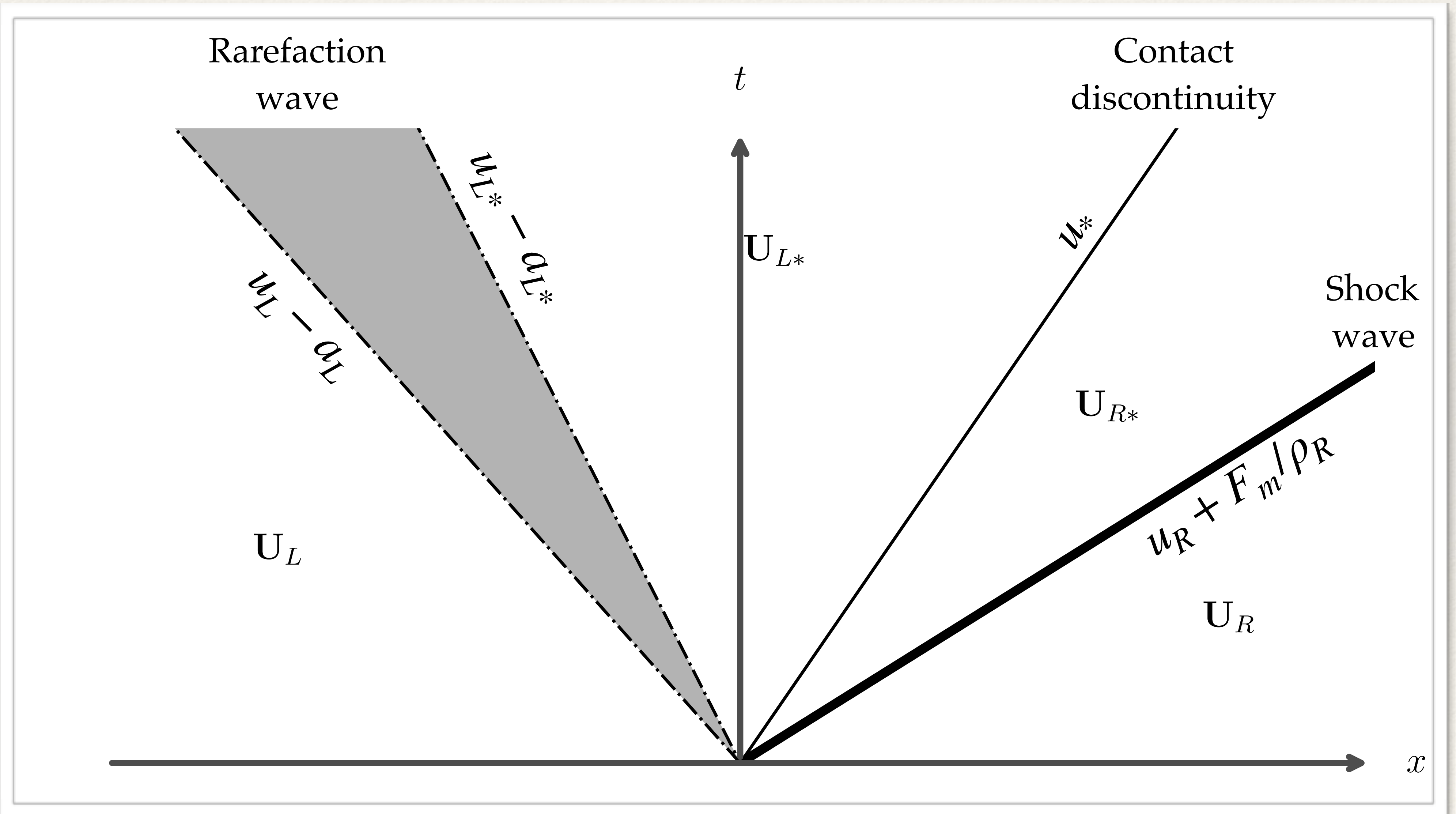
$$\begin{pmatrix} dw = \text{downwind} \\ uw = \text{upwind} \end{pmatrix}$$

$$\rho_{\mathrm{dw}} u_{\mathrm{dw}} = \rho_{\mathrm{uw}} u_{\mathrm{uw}} = F_m$$
$$\rho_{\mathrm{dw}} u_{\mathrm{dw}}^2 + p_{\mathrm{dw}} = \rho_{\mathrm{uw}} u_{\mathrm{uw}}^2 + p_{\mathrm{uw}} = F_p$$
$$F_m H_{\mathrm{dw}} = F_m H_{\mathrm{uw}} = F_E$$

The Riemann Problem

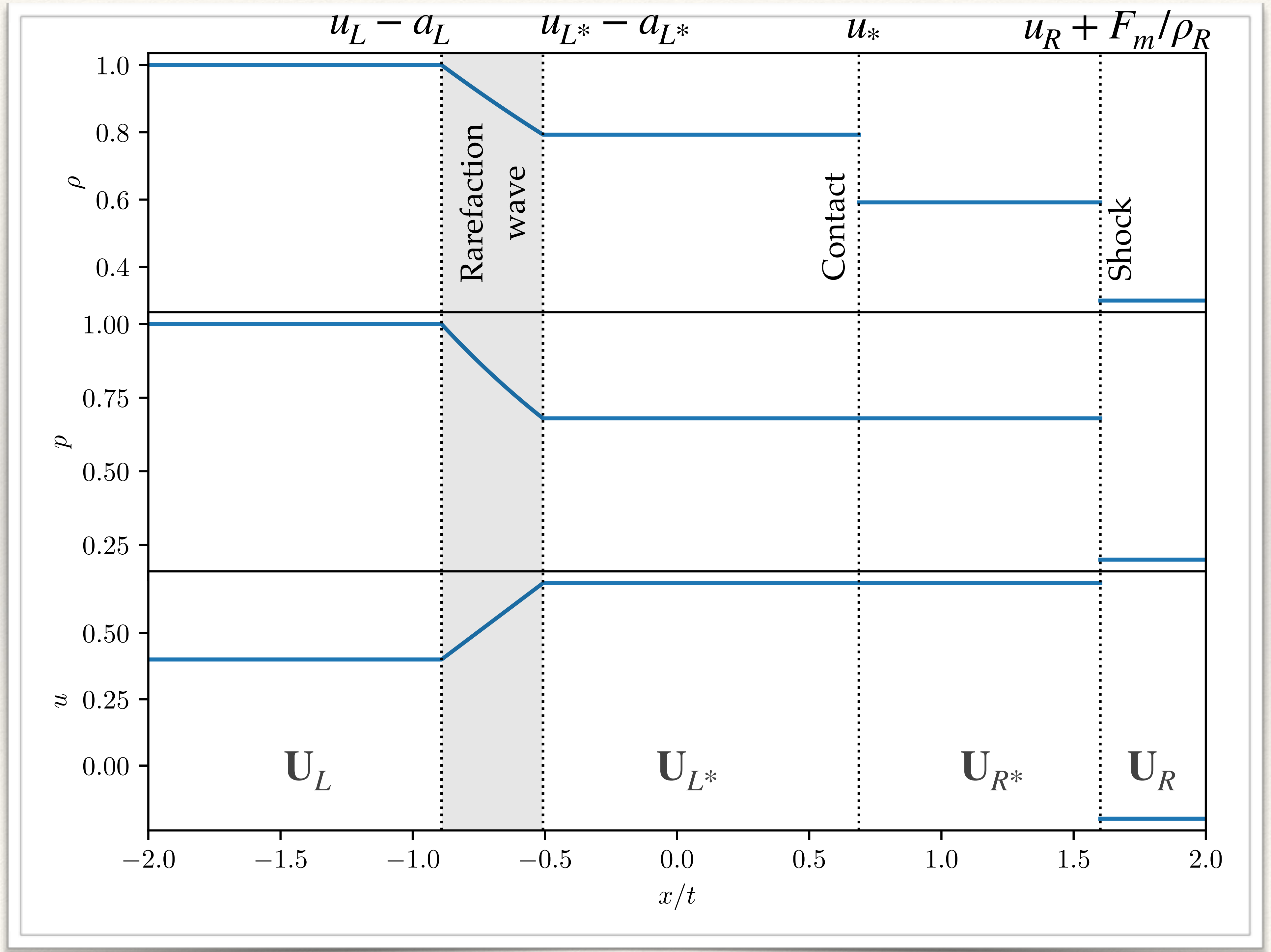
Solution

$\mathbf{U}(x,t) = \mathbf{U}(x/t)$



The Riemann Problem

Solution



Athena++ Implementation

Additional Functions

```
Real EquationOfState::PresFromRhoEg(Real rho, Real egas)
```

Gas pressure p | Density ρ | Gas energy density $e = \rho\epsilon$

```
Real EquationOfState::EgasFromRhoP(Real rho, Real pres)
```

Gas energy density e | Density ρ | Gas pressure p

```
Real EquationOfState::AsqFromRhoP(Real rho, Real pres)
```

(Sound speed)^2 a^2 | Density ρ | Gas pressure p

```
Real EquationOfState::RiemannAsq(Real rho, Real hint)
```

(Sound speed)^2 a^2 | Density ρ | hint=(egas+pres)/rho $(p + e)/\rho$

Athena++ Implementation

Additional Functions

$$p = (\gamma - 1)e \;\rightarrow\; p = p(\rho, e)$$

```
p = peos->PresFromRhoEg(rho, egas)
```

$$e = \frac{p}{\gamma - 1} \;\rightarrow\; e = e(\rho, p)$$

```
e = peos->EgFromRhoP(rho, pres)
```

$$a^2 = \gamma \frac{p}{\rho} \;\rightarrow\; a^2 = (\rho, p)$$

```
asq = peos->AsqFromRhoP(rho, pres)
```

$$a^2 = (\gamma - 1)\frac{h}{\rho} \;\rightarrow\; a^2 = (\rho, h/\rho)$$

```
asq = peos->RiemannAsq(rho, hint)
```

Athena++ Implementation

```
> python configure.py --prob eos_test --eos general/eos_table
```

```
# Entries must be space separated.
#  n_var,  n_espec, n_rho
# (fields) (rows)  (columns)
4 2 3
# Log espec lim (specific internal energy e/rho)
-1.0000e+01 2.0000e+01
# Log rho lim
-2.4000e+01 4.0000e+00
# Ratios = 1, eint/pres, eint/pres, eint/h
# This line is required iff EOS_read_ratios
1.0000e+00 1.0000e+01 1.0000e+01 9.0909e-01
# Log p/e(e/rho,rho)
-1.0000e+00 -1.0000e+00 -1.0000e+00
-1.0000e+00 -1.0000e+00 -1.0000e+00
# Log e/p(p/rho,rho)
1.0000e+00 1.0000e+00 1.0000e+00
1.0000e+00 1.0000e+00 1.0000e+00
# Log asq*rho/p(p/rho,rho)
4.1393e-02 4.1393e-02 4.1393e-02
4.1393e-02 4.1393e-02 4.1393e-02
# Log asq*rho/h(h/rho,rho)
-1.0000e+00 -1.0000e+00 -1.0000e+00
-1.0000e+00 -1.0000e+00 -1.0000e+00
```

Ideal EOS: $\gamma = 1.1$

$N_{\text{var}}, N_\epsilon, N_\rho$

$\log(\epsilon_{\min}), \log(\epsilon_{\max}) \quad \epsilon \equiv e/\rho$

$\log(\rho_{\min}), \log(\rho_{\max}) \quad \log(x) \equiv \log_{10}(x)$

$$\log\left[\frac{p}{e}(\epsilon, \rho)\right]$$

$$\log\left[\frac{e}{p}(p/\rho, \rho)\right]$$

$$\log\left[\frac{a^2\rho}{p}(p/\rho, \rho)\right] \quad a^2 \equiv \left(\frac{\partial p}{\partial \rho}\right)_s$$

$$\log\left[\frac{a^2\rho}{h}(h/\rho, \rho)\right] \quad h \equiv e + p$$

Example EOS

Simple Hydrogen EOS

```
> python configure.py --prob shock_tube --eos general/hydrogen
```

$$\mathrm{H}^0 \rightleftharpoons \mathrm{H}^+ + e^-$$

Saha equation:

$$\underbrace{1-x}_{\text{Neutral Fraction}} = x\frac{n_e Z_{H,0}}{Z_e Z_{H,1}} = x^2 \frac{\rho Z_{H,0}}{Z_e Z_{H,1}}$$

$$= x^2 \frac{\rho}{m_p n_q} \exp\left(\frac{T_{\rm ion}}{T}\right)\left(\frac{T_{\rm ion}}{T}\right)^{3/2}$$

$$p = \rho k T \left[1 + x(\rho, T)\right]$$

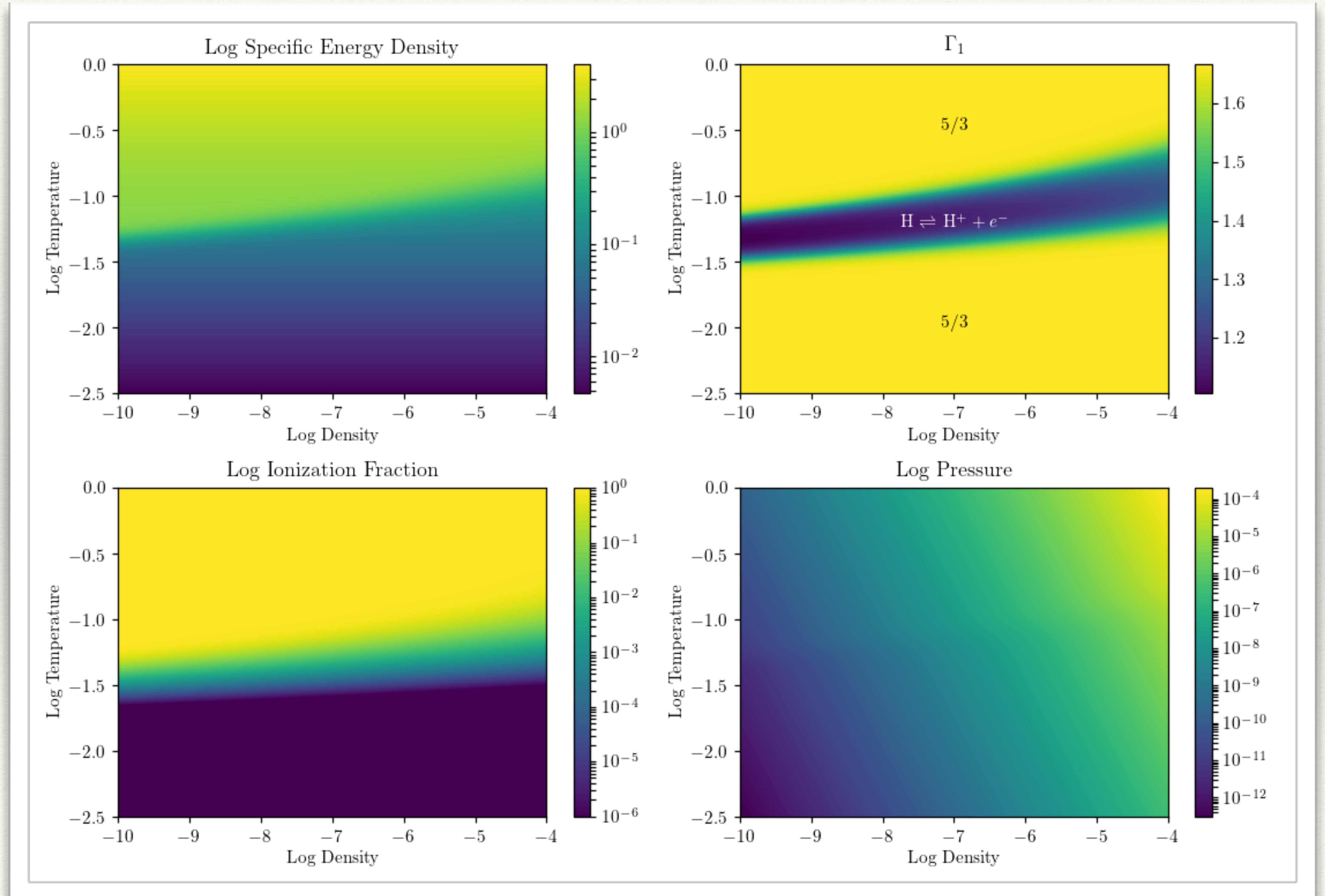
$$\epsilon = \frac{kT_{\rm ion}}{m_p} x(\rho, T) + \frac{3}{2}\frac{P}{\rho}$$

Table 1. Assumed Units

Quntity	Symbol	Expression	cgs value
mass	m_p	m_p	1.6726219e-24
number density	$n_{\rm q}$	$\left(\frac{2\pi m_e k T_{\rm ion}}{h^2}\right)^{3/2}$	1.514892e23
temperature	$T_{\rm ion}$	$\frac{1}{k}\frac{\alpha^2 m_e c^2}{2}$	157,888
density	$\rho_{\rm u}$	$m_p n_{\rm q}$	0.253384
pressure	$P_{\rm u}$	$n_{\rm q} k T_{\rm ion}$	3.302272e12
speed	$v_{\rm u}$	$\sqrt{kT_{\rm ion}/m_p}$	3.6100785e6
length	$x_{\rm u}$	$n_{\rm q}^{-1/3}$	1.8758844e-8
time	$t_{\rm u}$	$x_{\rm u}/v_{\rm u}$	5.196243e-15

Example EOS

Simple Hydrogen EOS

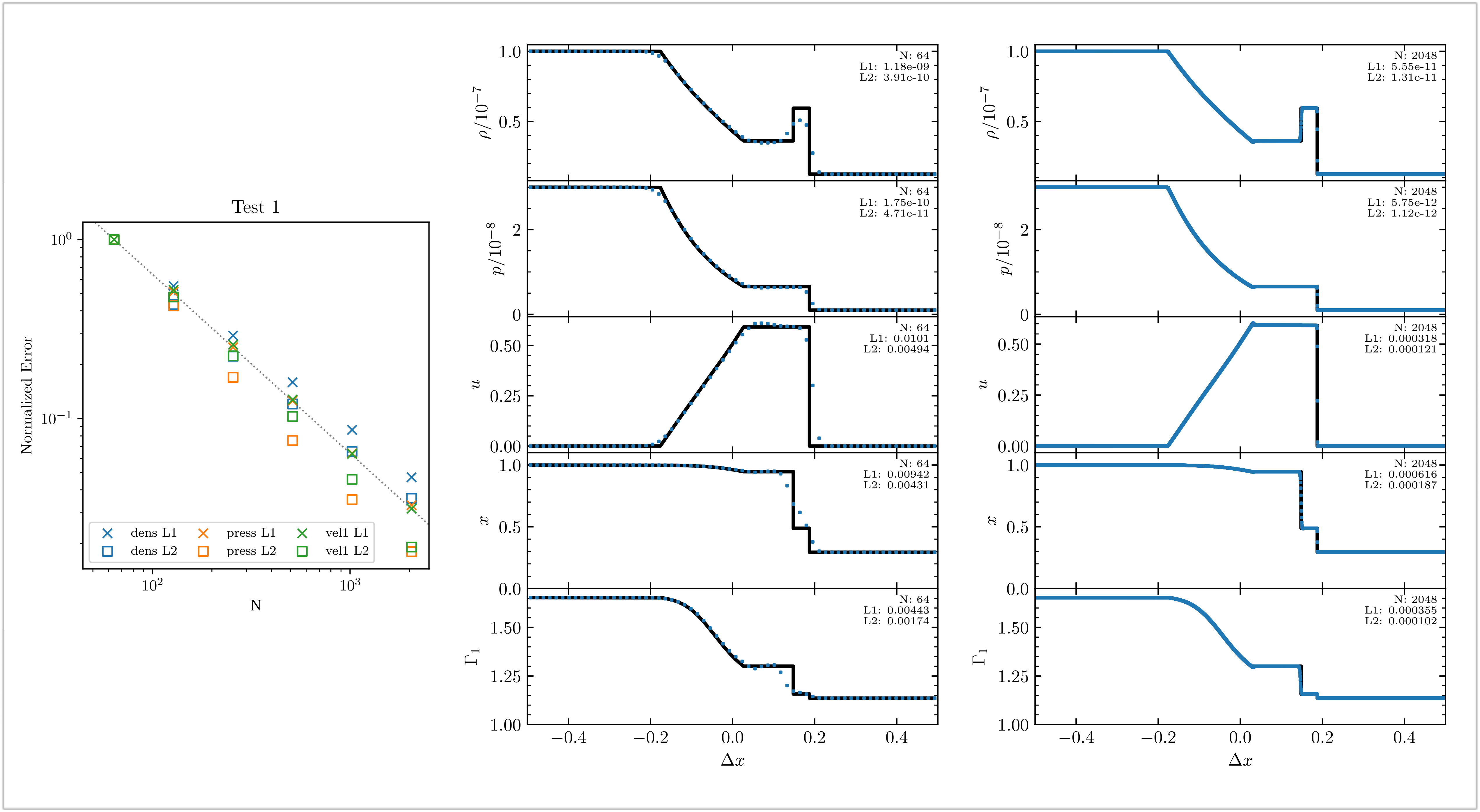


Tests

Table 2. Riemann Tests

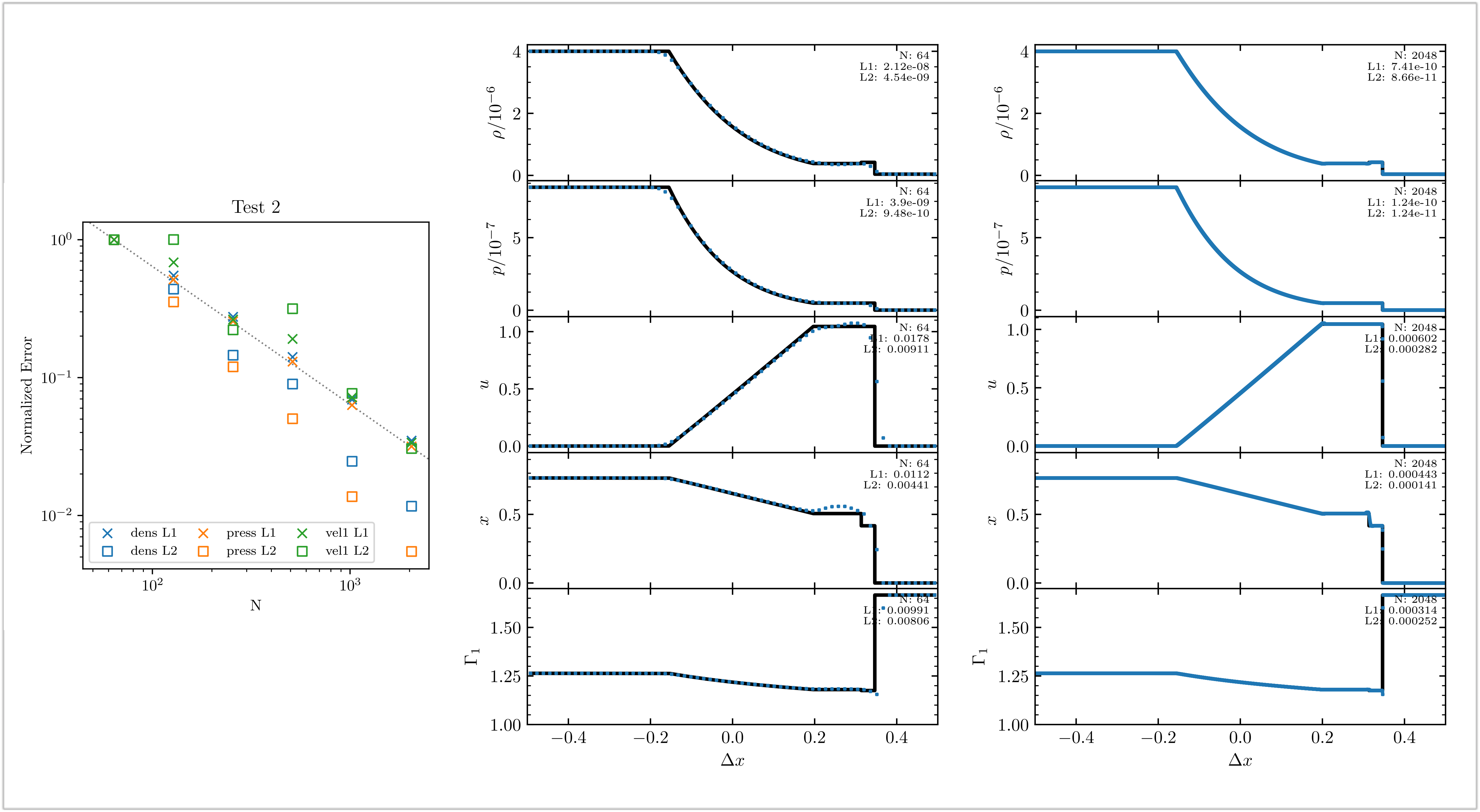
Test #	Test Type	ρ_l	u_l	T_l	ρ_r	u_r	T_r	$\Delta t/\Delta x$
1	Sod-like	1e-07	0.0	0.15	1.25e-08	0.0	0.062	0.25
2	Sod-like	4e-06	0.0	0.12	4e-08	0.0	0.019	0.3
3	Asym. Shock-Shock	8e-07	1.1	0.006	4e-07	-1.7	0.006	1.5
4	Asym. Shock-Shock	5e-07	1.5	0.006	4e-07	-1.8	0.006	1.5
5	Sym. Rare-Rare	8e-05	-0.8	0.095	8e-05	0.8	0.095	0.25
6	Asym. Rare-Rare	6e-05	-0.5	0.095	8e-05	0.9	0.095	0.25

Test 1



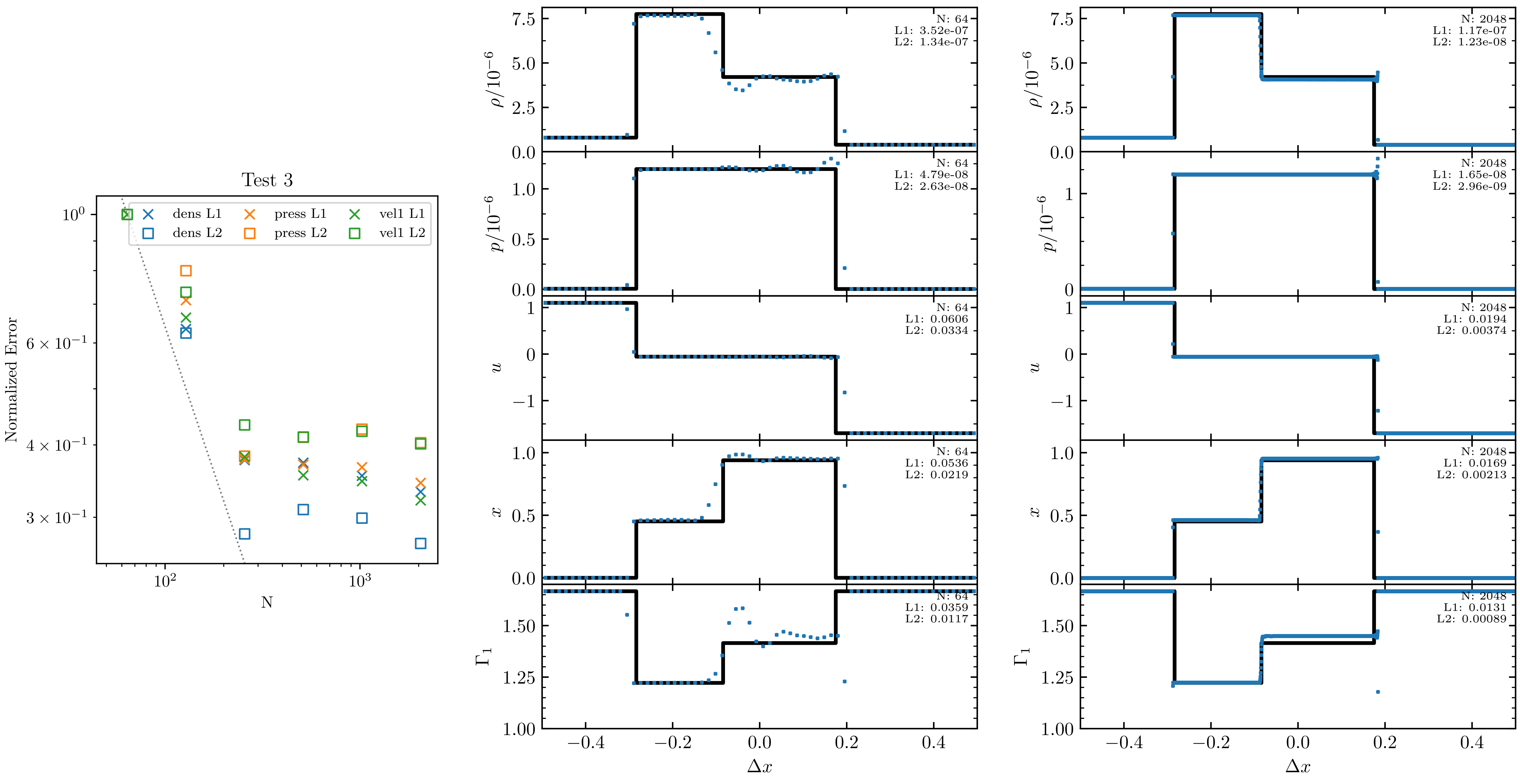
Test 1
Normalized Error
N
dens L1
dens L2
press L1
press L2
vel1 L1
vel1 L2
N: 64
L1: 1.18e-09
L2: 3.91e-10
N: 64
L1: 1.75e-10
L2: 4.71e-11
N: 64
L1: 0.0101
L2: 0.00494
N: 64
L1: 0.00942
L2: 0.00431
N: 64
L1: 0.00443
L2: 0.00174
N: 2048
L1: 5.55e-11
L2: 1.31e-11
N: 2048
L1: 5.75e-12
L2: 1.12e-12
N: 2048
L1: 0.000318
L2: 0.000121
N: 2048
L1: 0.000616
L2: 0.000187
N: 2048
L1: 0.000355
L2: 0.000102
$\rho/10^{-7}$
$p/10^{-8}$
u
x
Γ_1
Δx

Test 2



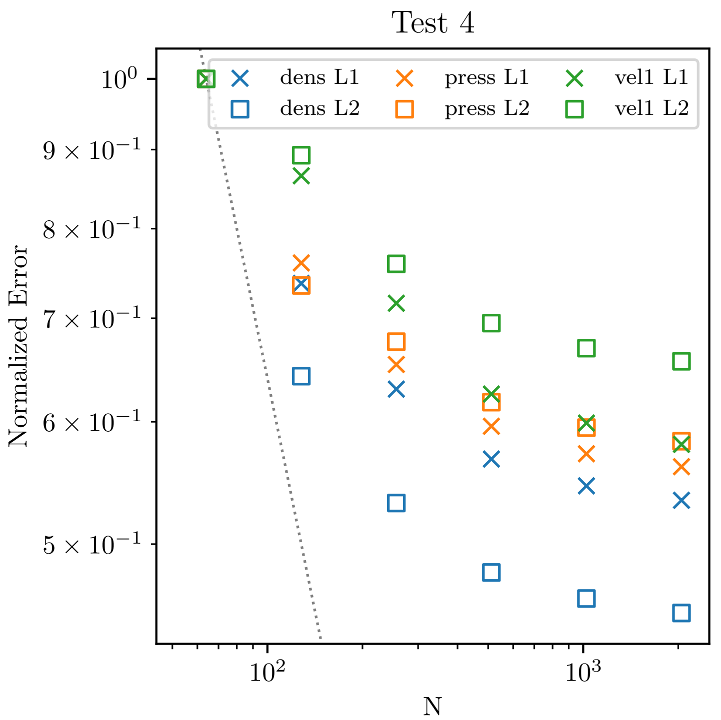
Test 2
Normalized Error
N
dens L1
dens L2
press L1
press L2
vel1 L1
vel1 L2
N: 64
L1: 2.12e-08
L2: 4.54e-09
N: 2048
L1: 7.41e-10
L2: 8.66e-11
N: 64
L1: 3.9e-09
L2: 9.48e-10
N: 2048
L1: 1.24e-10
L2: 1.24e-11
N: 64
L1: 0.0178
L2: 0.00911
N: 2048
L1: 0.000602
L2: 0.000282
N: 64
L1: 0.0112
L2: 0.00441
N: 2048
L1: 0.000443
L2: 0.000141
N: 64
L1: 0.00991
L2: 0.00806
N: 2048
L1: 0.000314
L2: 0.000252
$\rho/10^{-6}$
$p/10^{-7}$
u
x
Γ_1
Δx

Test 3

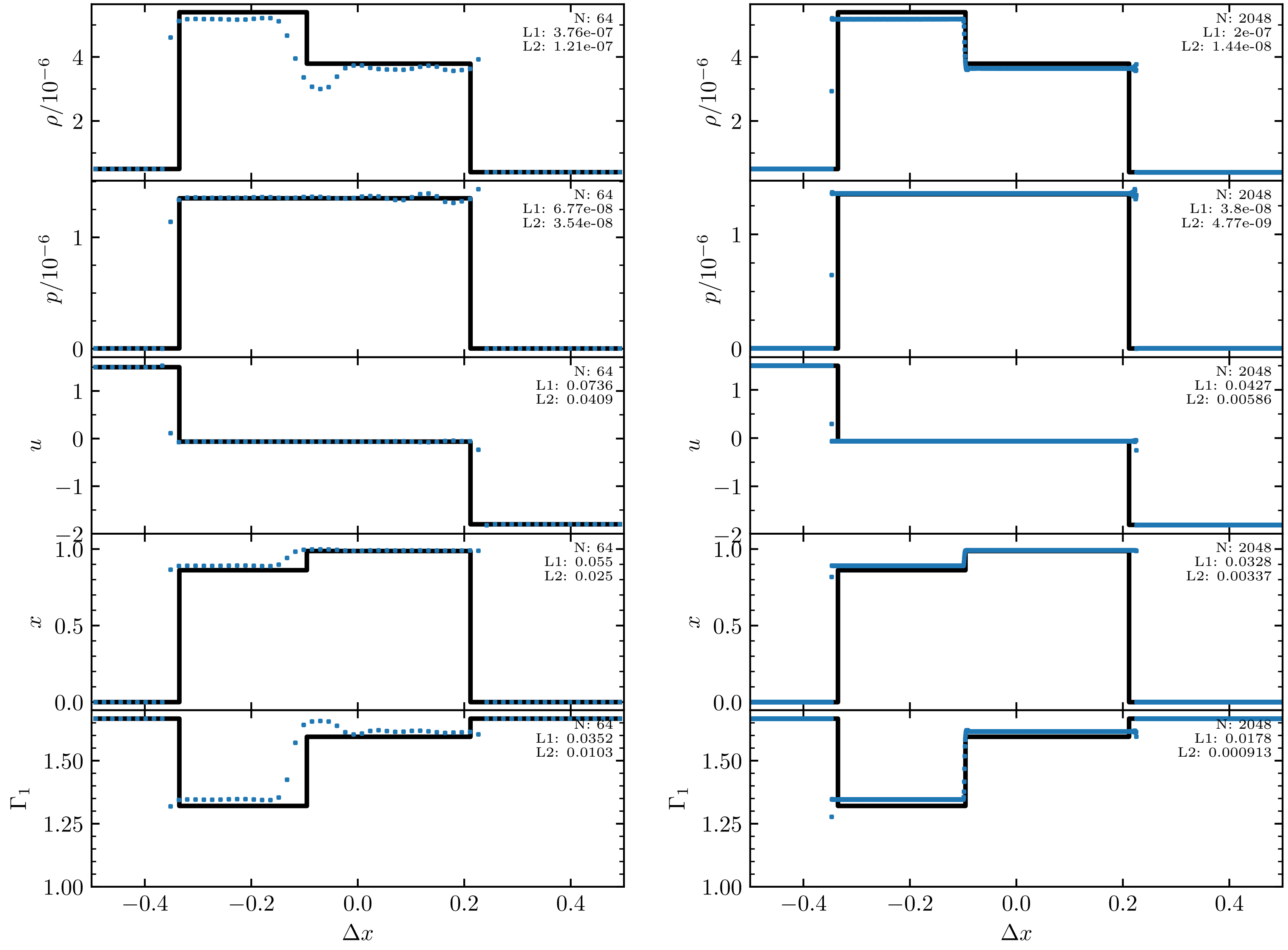


Test 3
dens L1
dens L2
press L1
press L2
vel1 L1
vel1 L2
Normalized Error
N
N: 64
L1: 3.52e-07
L2: 1.34e-07
N: 64
L1: 4.79e-08
L2: 2.63e-08
N: 64
L1: 0.0606
L2: 0.0334
N: 64
L1: 0.0536
L2: 0.0219
N: 64
L1: 0.0359
L2: 0.0117
N: 2048
L1: 1.17e-07
L2: 1.23e-08
N: 2048
L1: 1.65e-08
L2: 2.96e-09
N: 2048
L1: 0.0194
L2: 0.00374
N: 2048
L1: 0.0169
L2: 0.00213
N: 2048
L1: 0.0131
L2: 0.00089
$\rho/10^{-6}$
$p/10^{-6}$
u
x
Γ_1
Δx

Test 4

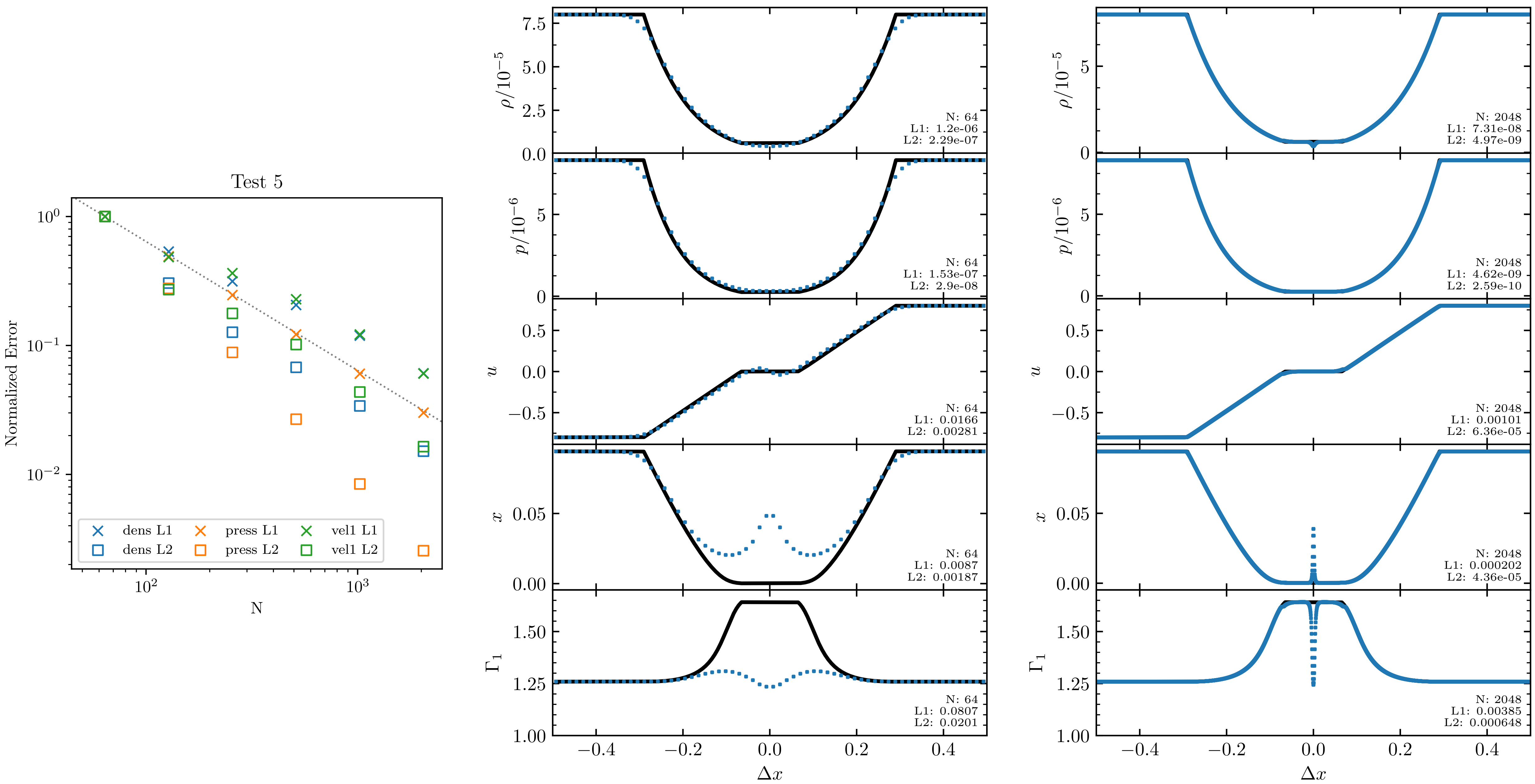


Test 4
Normalized Error
N
dens L1
dens L2
press L1
press L2
vel1 L1
vel1 L2



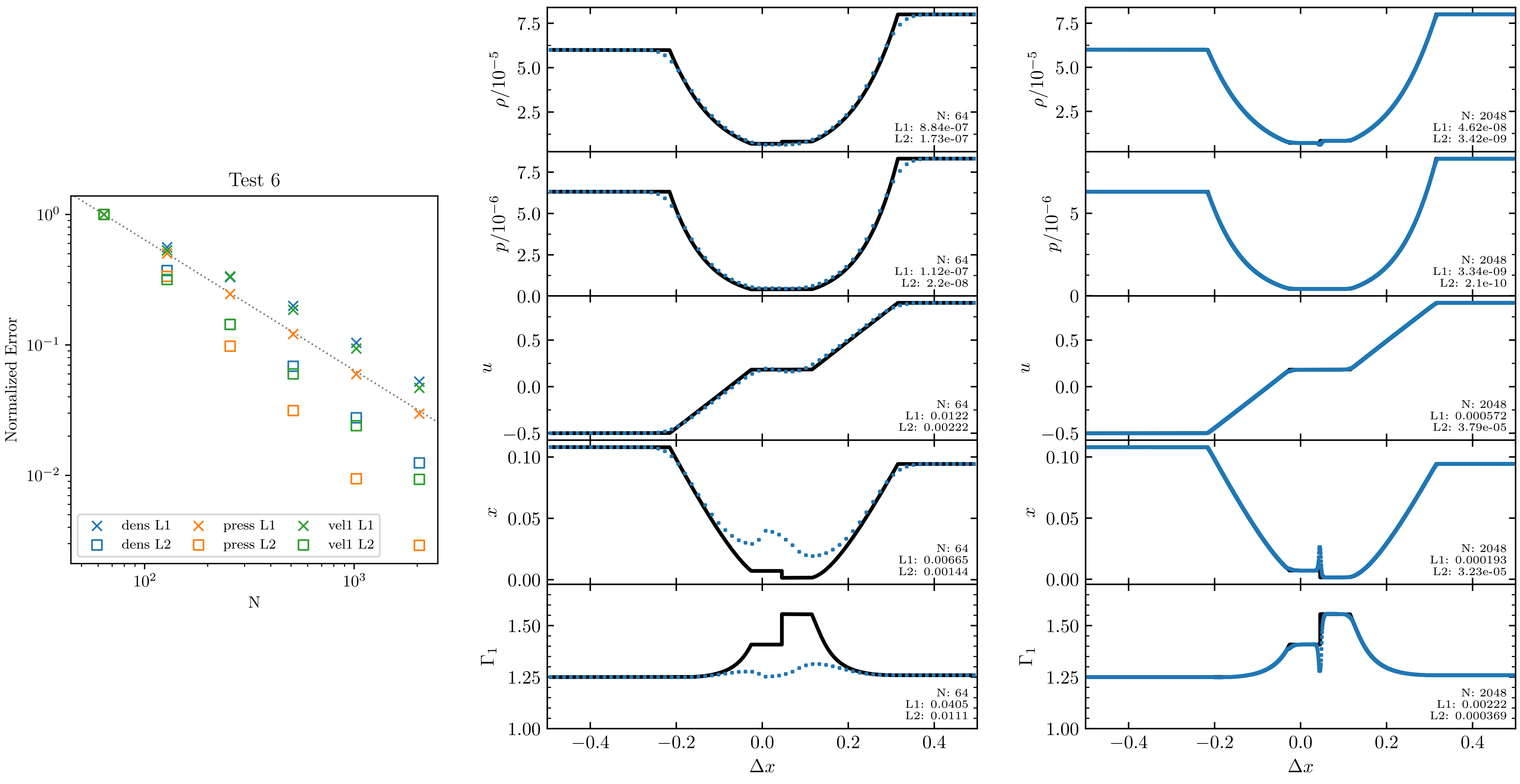
N: 64
L1: 3.76e-07
L2: 1.21e-07
N: 64
L1: 6.77e-08
L2: 3.54e-08
N: 64
L1: 0.0736
L2: 0.0409
N: 64
L1: 0.055
L2: 0.025
N: 64
L1: 0.0352
L2: 0.0103
N: 2048
L1: 2e-07
L2: 1.44e-08
N: 2048
L1: 3.8e-08
L2: 4.77e-09
N: 2048
L1: 0.0427
L2: 0.00586
N: 2048
L1: 0.0328
L2: 0.00337
N: 2048
L1: 0.0178
L2: 0.000913
Δx

Test 5



Test 5
Normalized Error
N
dens L1
dens L2
press L1
press L2
vel1 L1
vel1 L2
N: 64
L1: 1.2e-06
L2: 2.29e-07
N: 64
L1: 1.53e-07
L2: 2.9e-08
N: 64
L1: 0.0166
L2: 0.00281
N: 64
L1: 0.0087
L2: 0.00187
N: 64
L1: 0.0807
L2: 0.0201
N: 2048
L1: 7.31e-08
L2: 4.97e-09
N: 2048
L1: 4.62e-09
L2: 2.59e-10
N: 2048
L1: 0.00101
L2: 6.36e-05
N: 2048
L1: 0.000202
L2: 4.36e-05
N: 2048
L1: 0.00385
L2: 0.000648
$\rho/10^{-5}$
$p/10^{-6}$
u
x
Γ_1
Δx

Test 6



Test 6
Normalized Error
N
dens L1
dens L2
press L1
press L2
vel1 L1
vel1 L2
$\rho/10^{-5}$
$p/10^{-6}$
u
x
Γ_1
Δx
N: 64
L1: 8.84e-07
L2: 1.73e-07
N: 64
L1: 1.12e-07
L2: 2.2e-08
N: 64
L1: 0.0122
L2: 0.00222
N: 64
L1: 0.00665
L2: 0.00144
N: 64
L1: 0.0405
L2: 0.0111
N: 2048
L1: 4.62e-08
L2: 3.42e-09
N: 2048
L1: 3.34e-09
L2: 2.1e-10
N: 2048
L1: 0.000572
L2: 3.79e-05
N: 2048
L1: 0.000193
L2: 3.23e-05
N: 2048
L1: 0.00222
L2: 0.000369

Summary

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Future Goals

- MHD (need tests)
- Function of passive scalers
- More table options?
- Implement HLLE
- SR/GR
- Add temperature function

Assumptions

$$\left(\frac{\partial p}{\partial \rho}\right)_\epsilon > 0, \quad \left(\frac{\partial p}{\partial \epsilon}\right)_\rho > 0$$

One Thermodynamic Derivative

$$a^2 = \left(\frac{\partial p}{\partial \rho}\right)_s$$

Additional Functions

```
Real EquationOfState::PresFromRhoEg(Real rho, Real egas)
```

Gas pressure p — Density ρ — Gas energy density $e = \rho\epsilon$

```
Real EquationOfState::EgasFromRhoP(Real rho, Real pres)
```

Gas energy density e — Density ρ — Gas pressure p

```
Real EquationOfState::AsqFromRhoP(Real rho, Real pres)
```

(Sound speed)^2 a^2 — Density ρ — Gas pressure p

```
Real EquationOfState::RiemannAsq(Real rho, Real hint)
```

(Sound speed)^2 a^2 — Density ρ — hint=(egas+pres)/rho $(p + e)/\rho$

Wiki

https://github.com/PrincetonUniversity/athena/wiki/General-Equation-of-State