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Discontinuity-Aware Solvers for Vapor-Compression Cycles

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Motivation

- The behavior of many physical systems have derivative discontinuities
  - Collisions; condensation / evaporation

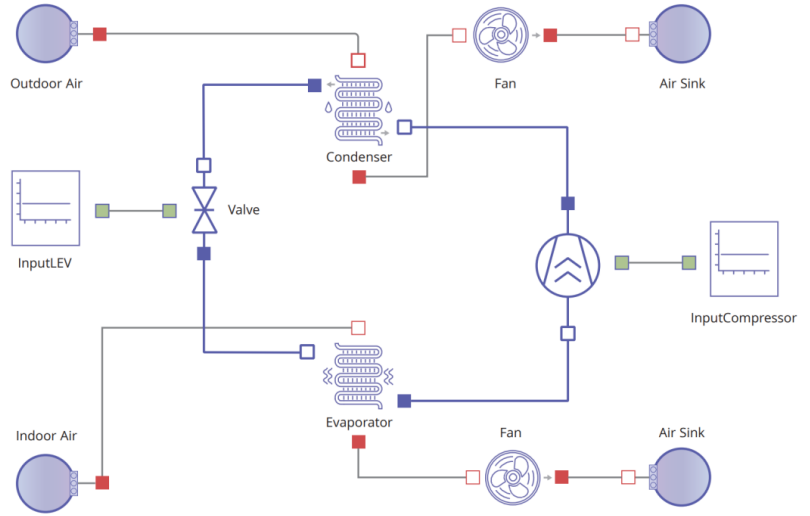


- These discontinuities can present challenges when solving DAEs
  - Solver slows down whenever a discontinuities are crossed
  - Discontinuities are an implicit function of the states; $h_{bub}(P)$
  - These discontinuities are best expressed in modeling equations

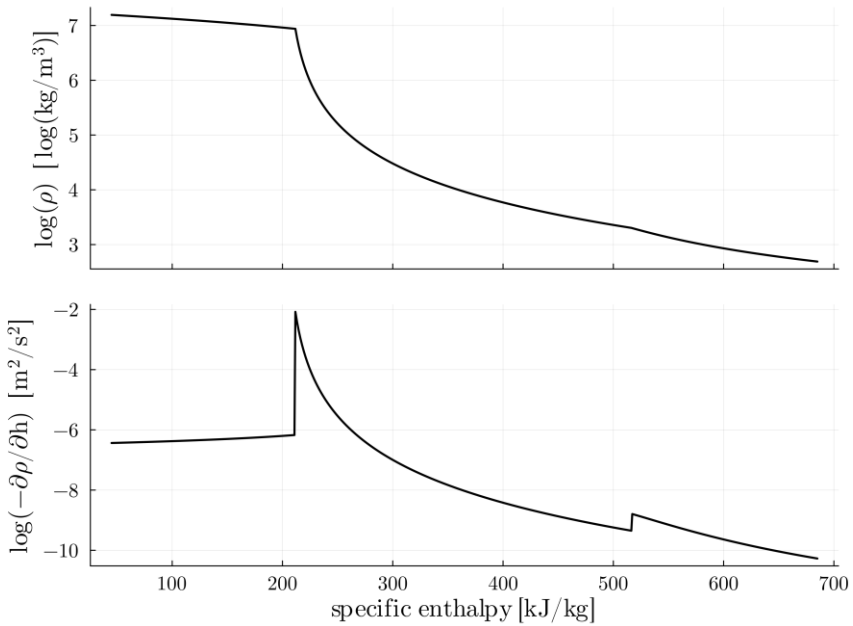
Questions:

- Can we automatically pass this information from the models to the solvers?
- Do the simulations run faster if the solver knows about these discontinuities a priori?

Vapor compression cycle



Derivative discontinuities at the bubble/dew points



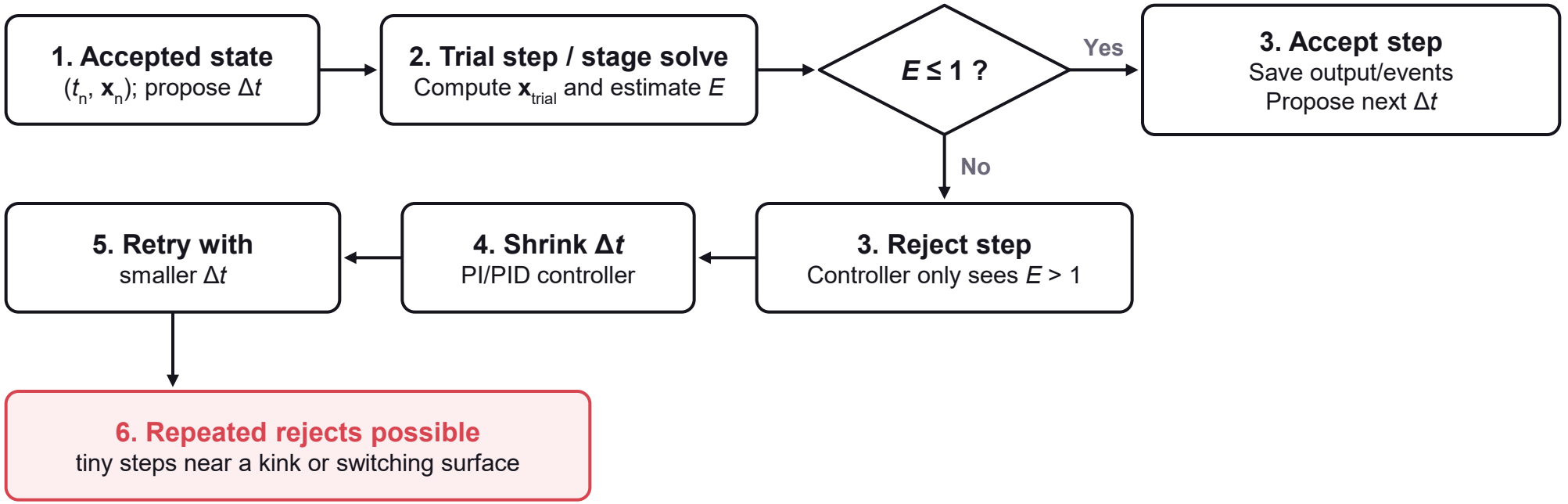
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Previous Work

- **Carver (1978); Cellier (1979):** mark discontinuities with zero-crossing functions
- **Gustafsson (1994):** step to the discontinuity instead of rejecting repeatedly
- **Park & Barton (1996):** interval arithmetic guarantees no crossing is missed
- **Otter et al. (1999):** Modelica treats every relation as a potential state event
- **Fredriksson et al. (2014):** integrator-independent, domain-based events (Assimulo)

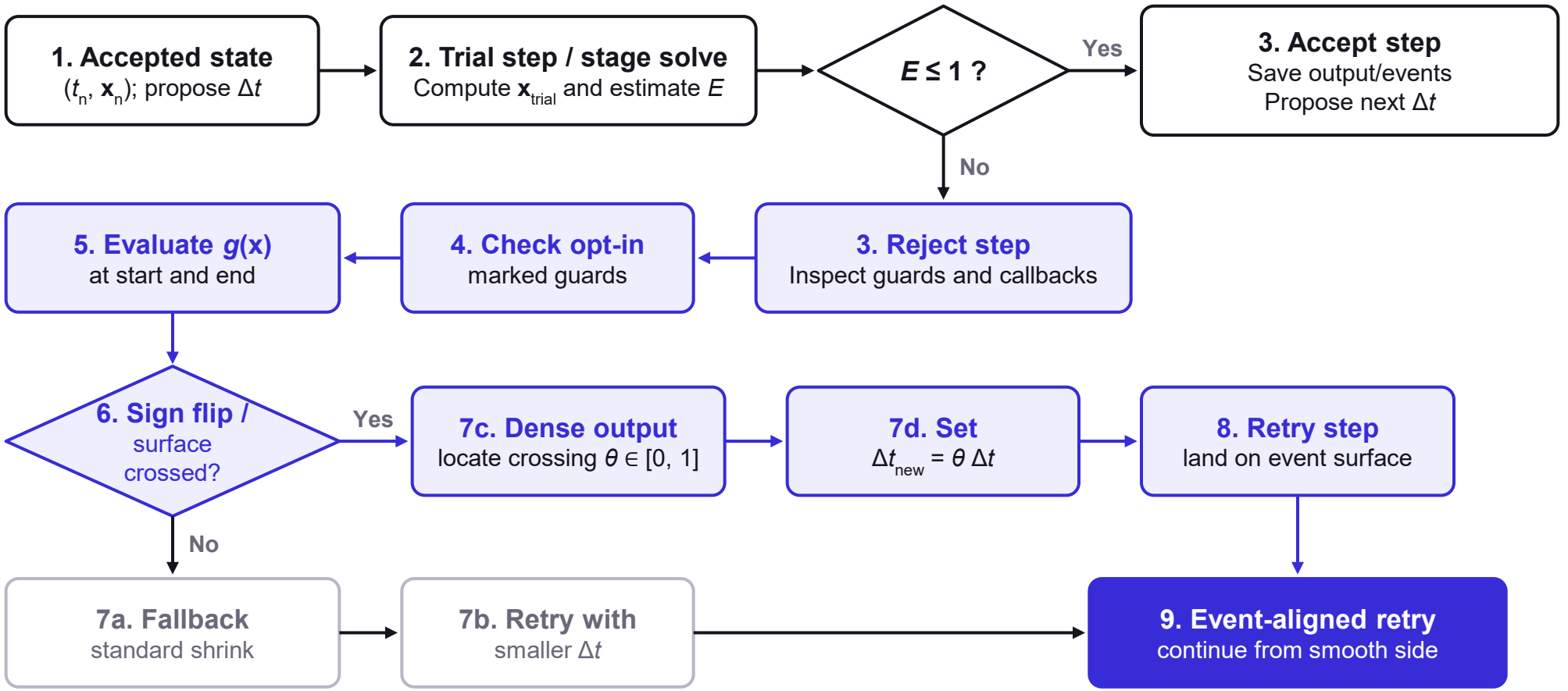
> **Contribution:** Leverage user-declared information to compute appropriate step sizes. Use zero-crossing functions to locate discontinuities on rejected steps, not just accepted ones

Standard Step-Size Control



Step 4 shrinks Δt from the error estimate alone, e.g. $h_{new} = f_{safe} \cdot h / E^{1/(p+1)}$, so it cannot see where the kink is.

Discontinuity-Aware Step-Size Control

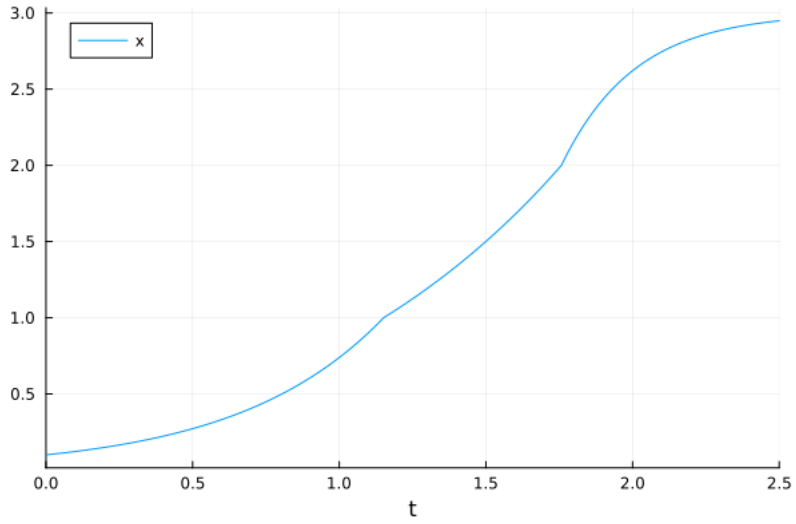


Highlighted: what changes on a rejected step. With no sign change, it falls back to the standard shrink (7a–7b).

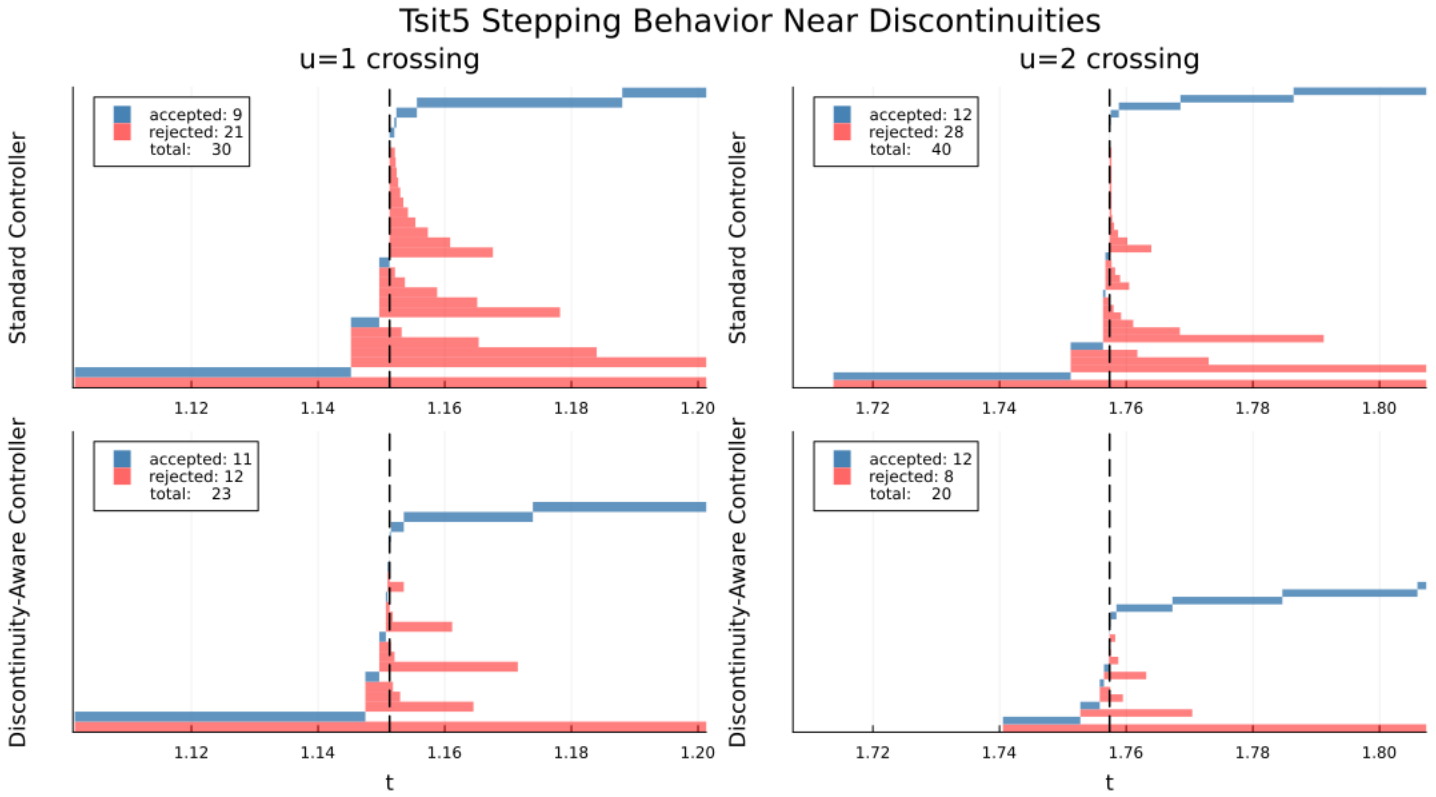
Test Problem 1: Scalar ODE with Two Kinks

$$\dot{x} = \begin{cases} 2x, & x < 1 \\ x + 0.2, & 1 \leq x < 2 \\ -4x + 12, & x \geq 2 \end{cases}$$

- $x(0) = 0.1$, $t \in [0, 2.5]$
- `Tsit5` (explicit) and `Rodas5P` (Rosenbrock)

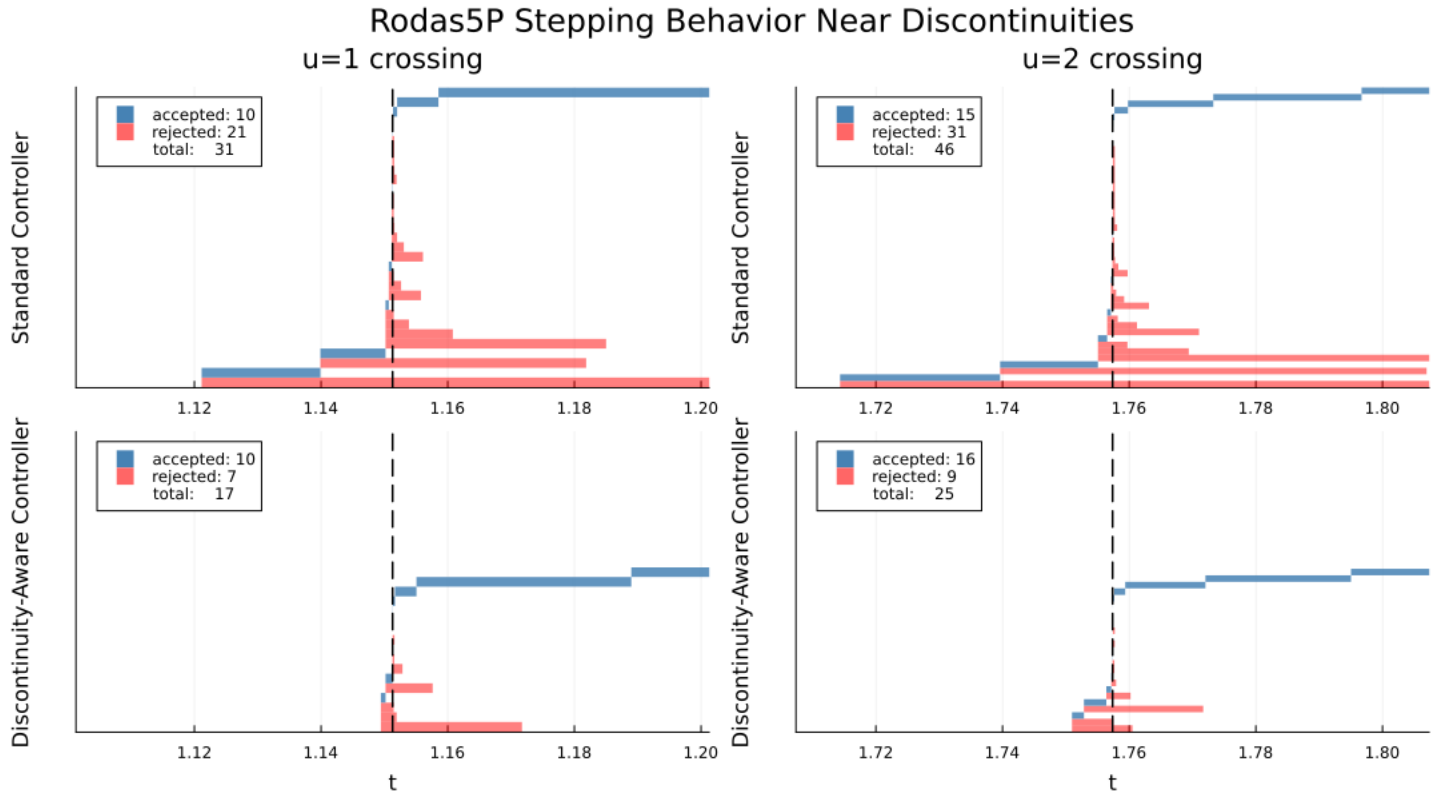


Tsit5: Fewer Rejected Steps at each Kink



– Rejected steps: 21 → 12 at $x = 1$, and 28 → 8 at $x = 2$ (top: standard, bottom: discontinuity-aware)

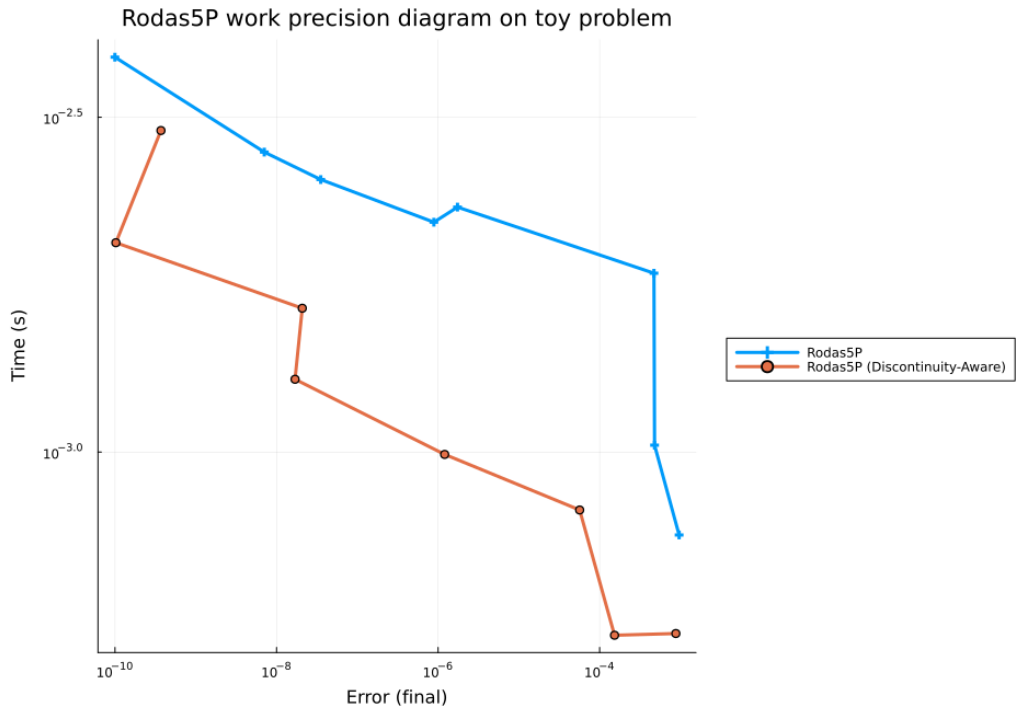
Rodas5P: Fewer Rejected Steps at each Kink



– Rejected steps: 21 → 7 at $x = 1$, and 31 → 9 at $x = 2$

Test Problem 1: Faster at every Tolerance

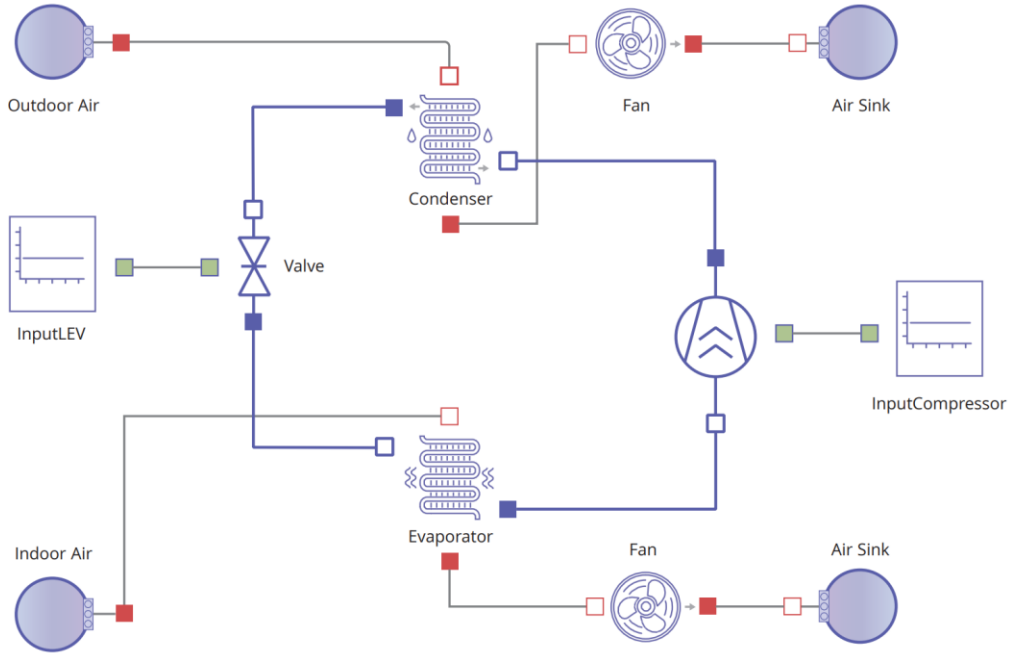




– Larger gain for `Rodas5P`: rejected steps cost more for an implicit method

Dyad HVAC

- **Pre-built components** — tube-fin and plate heat exchangers; compressors, valves, fans, pipes
  - 8 volumes/HEX in this model
- **Thermodynamic property models** — spline-based refrigerants, dry and moist air
  - Zero-crossing functions to mark discontinuities
- **Ecosystem** — numerical solvers; calibration, machine learning, control



1D Refrigerant Flow Model

$$\frac{\partial(\rho A)}{\partial t} + \frac{\partial(\rho A v)}{\partial x} = 0$$
$$\frac{\partial(\rho v A)}{\partial t} + \frac{\partial(\rho v^2 A)}{\partial x} = -A\frac{\partial p}{\partial x} - F_f$$
$$\frac{\partial(\rho u A)}{\partial t} + \frac{\partial(\rho v h A)}{\partial x} = vA\frac{\partial p}{\partial x} + vF_f + \frac{\partial Q}{\partial x}$$

Heat Exchangers dominate dynamics

3D Air Flow Model

$$\frac{\partial(\rho_a v_a c_{p,a} T_a)}{\partial z} = \alpha(T_w - T_a)\frac{\partial^2 A_e}{\partial x \partial y}$$
$$\frac{\partial(\rho_a v_a \omega_a)}{\partial z} = \frac{\alpha}{Le^{2/3} c_{p,a}}(\omega_{w,s} - \omega_a)\frac{\partial^2 A_e}{\partial x \partial y}$$
$$\rho_w c_w \frac{\partial T_w}{\partial t} = k\nabla^2 T_w + \sum q'''$$

Fast and Accurate B-spline models

Algebraic Compressor Model

$$\eta_v(f, p_r, \ldots) = \frac{\dot{m}_{\text{comp}}}{\rho_{\text{suc}} V_f}$$
$$\eta_{is}(f, \ldots) = \frac{h_{\text{dis,isen}} - h_{\text{suc}}}{h_{\text{dis}} - h_{\text{suc}}}$$

Compressor and Valve Performance curves

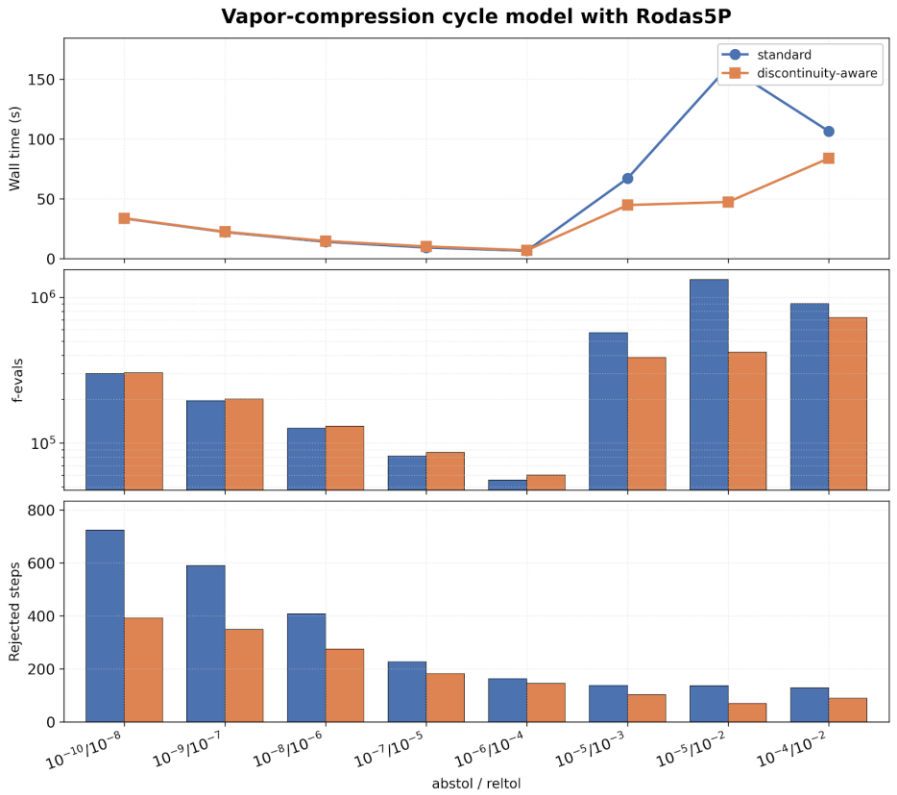
Algebraic LEV Model

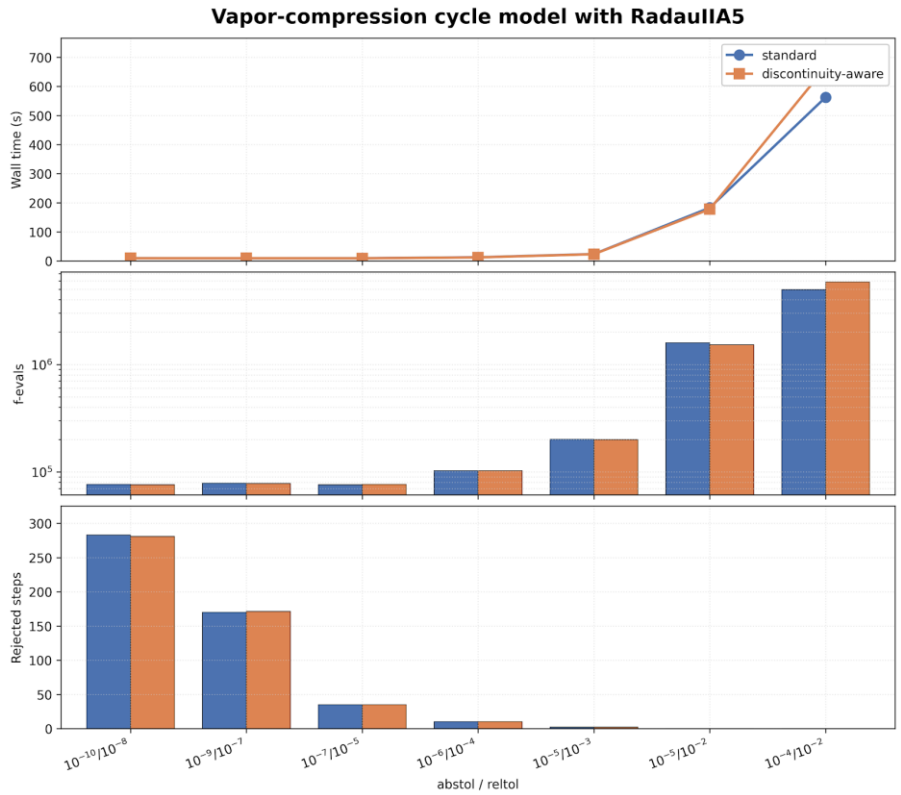
$$\dot{m} = C_v A_v \sqrt{\rho_{\text{in}} \Delta P}$$

Heat transfer, Pressure drop constituent relations.

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Test Problem 2: Rodas5P Gains at Loose Tolerances





- `Rodas5P` ~2× faster on average at loose tolerances; `RadauIIA5` essentially unchanged

Worst-Case Solve Times Shrink By Up To 8x

	MEDIAN		P75		P90		MAX	
abstol / reltol	ND	D	ND	D	ND	D	ND	D
Default	13.2	9.8	38.8	**13.3**	445.8	**81.5**	916.9	804.5
10^{-4} / 10^{-2}	42.0	69.1	132.2	117.1	168.5	170.4	651.3	**217.3**
10^{-5} / 10^{-2}	34.7	32.5	122.9	**50.0**	322.7	**98.8**	1245.9	**150.5**
10^{-5} / 10^{-3}	22.6	24.9	59.8	**27.8**	223.0	**30.5**	304.3	380.4
10^{-6} / 10^{-4}	6.3	6.9	6.4	7.0	6.9	7.2	9.4	7.6

`Rodas5P` solve time (s) over 15 runs. ND standard, D discontinuity-aware; **highlighted**: ≥2× faster. A 20-minute worst case finishes in 2.5.

Summary and Conclusions

- **Discontinuity-aware step control** — event information used on rejected steps too; open source in `DifferentialEquations.jl`
- **Declared in the model, used by the solver** — phase boundaries specified symbolically in Dyad, without reassembling the model
- **Largest gains for linearly implicit methods at loose tolerances** — `Rodas5P` up to 8x faster in the tails; fully implicit `RadauIIA5` is already robust
- **Not necessarily significantly better for tight tolerances** — but can be helpful for looser tolerances, so might be particularly relevant for distributed simulation architectures