

Hybrid theorem proving as a lightweight method for verifying numerical software

Alper Altuntas¹ John Baugh²

altuntas@ucar.edu, jwb@ncsu.edu

¹National Center for Atmospheric Research, Boulder, CO

²North Carolina State University, Raleigh, NC

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Numerical Software Verification

- ▶ The accuracy of physical models depend on:
 1. Convergence of numerical methods.
 2. Correctness of realization in software:
 - ▶ Complicated by intermittent discrete updates.
- ▶ This study presents:
 - ▶ A lightweight verification approach for (2).

Hybrid Theorem Proving

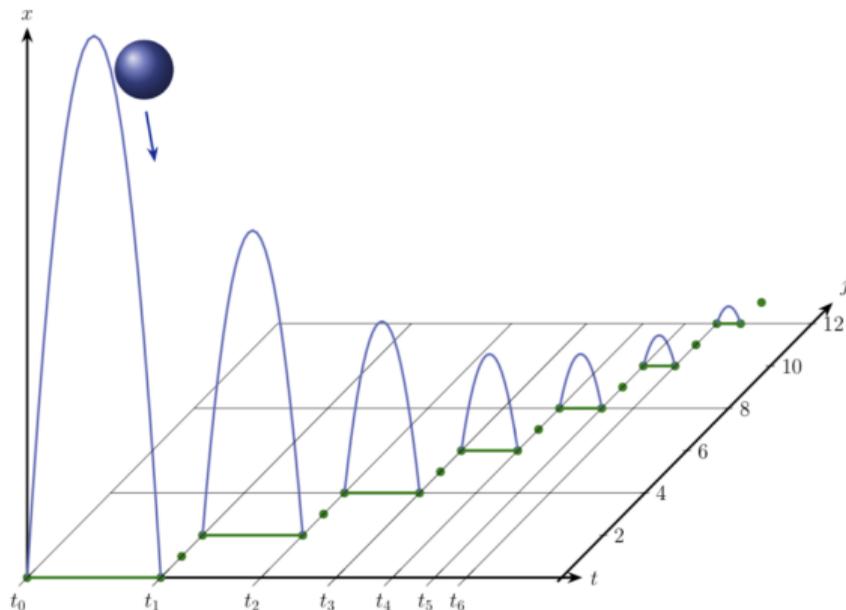
A formal verification technique for cyber-physical systems.

Hybrid Theorem Proving

- ▶ **Cyber-physical systems** are compositions of:
 1. Real world physics
continuous evolution
 2. Computer sampling (sensors) and intervention (actuators)
discrete changes
 - ▶ Examples: self-driving cars, ATC, robots, etc.
 - ▶ Verification tools: hybrid theorem provers, e.g., KeYmaera X
- ▶ **Hybrid programs** that model cyber-physical systems:
 1. ODEs model real world physics.
 2. Discrete programs model computer intervention.

Hybrid Theorem Proving

Continuous Evolution + Intermittent Discrete Changes



Platzer, A. "Logical Foundations of Cyber-Physical Systems." (2018)

- ▶ Continuous evolution:

$$\frac{\partial x}{\partial t} = v, \quad \frac{\partial v}{\partial t} = -g$$

- ▶ Discrete change:

$$v := -v$$

Hybrid Theorem Proving

A hybrid model:

$(0 \leq x \leq x_{max}) \rightarrow$	<i>initial conditions</i>
$[\{$	<i>execution begins</i>
$\{x' = v, v' = -g\}$	<i>continuous evolution</i>
$v := -v;$	<i>discrete assignment</i>
$\}^*$	<i>loop or terminate</i>
$(0 \leq x \leq x_{max})$	<i>postcondition</i>

where x is altitude, v is velocity, a is acceleration.

Hybrid Theorem Proving

A hybrid model:

	$(0 \leq x \leq x_{max}) \rightarrow$	<i>initial conditions</i>
	[{	<i>execution begins</i>
over some Δt {	$\{x' = v, v' = -g\}$	<i>continuous evolution</i>
instantaneous {	$v := -v;$	<i>discrete assignment</i>
	}*]	<i>loop or terminate</i>
	$(0 \leq x \leq x_{max})$	<i>postcondition</i>

where x is altitude, v is velocity, a is acceleration.

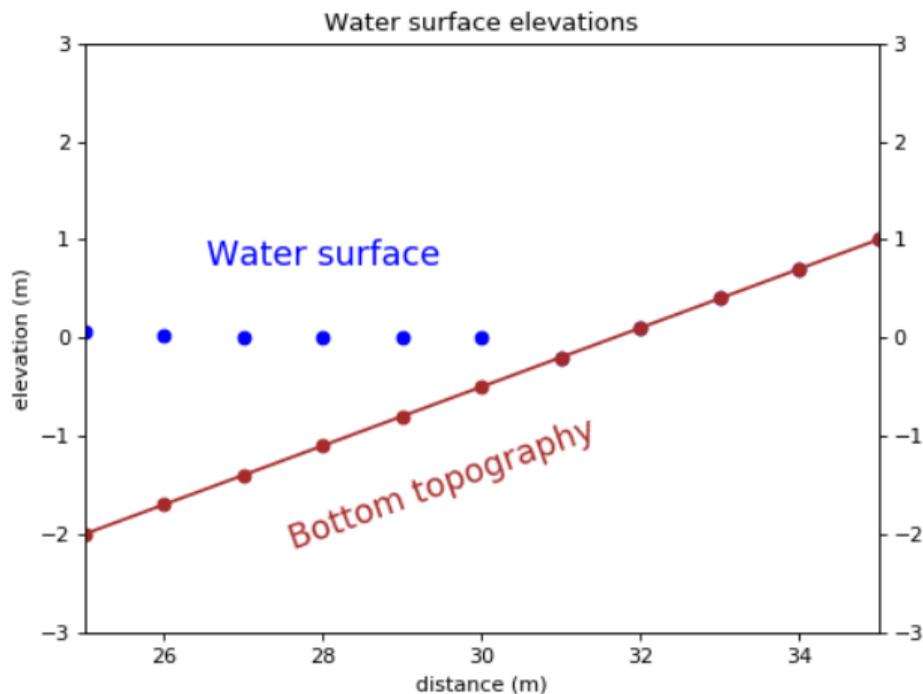
Hybrid theorem proving for verifying numerical software

A lightweight formal methods approach

Hybrid theorem proving for verifying numerical software

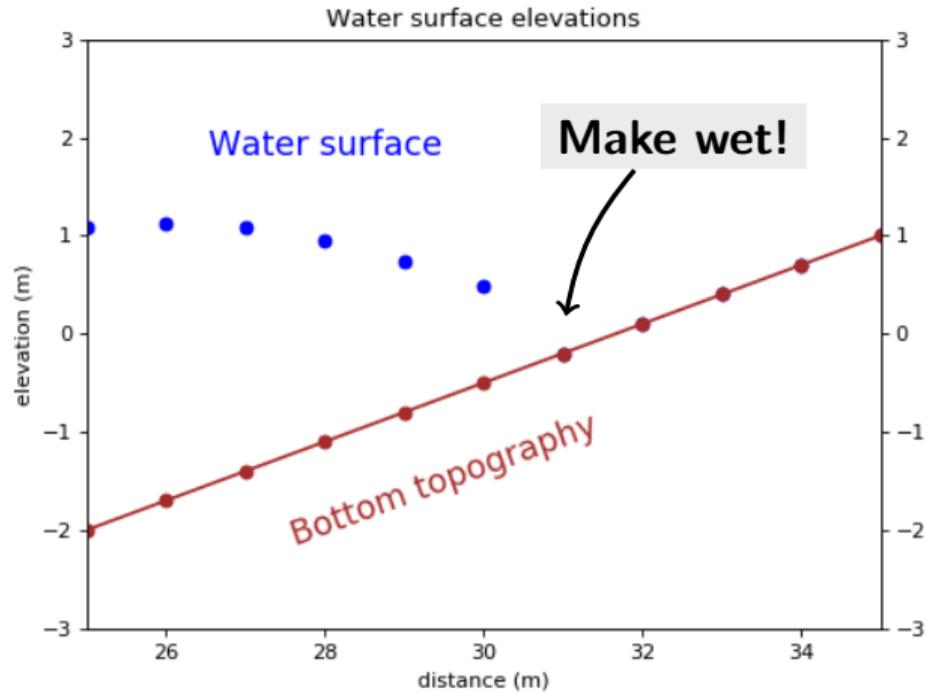
- ▶ Based on viewing numerical models as a hybrid system.
 1. **Continuous processes:** differential equations (DEs) solved by the model.
e.g., evolution of water surface height
 2. **Discrete updates:** often arise from ad-hoc and empirical modeling.
e.g., a location becoming wet/dry
- ▶ DEs are discretized in time and space, yet they may be taken to be continuous.
 - ▶ to abstract away from numerical methods.
 - ▶ to focus on discrete decisions and updates.

Hybrid theorem proving for verifying numerical software



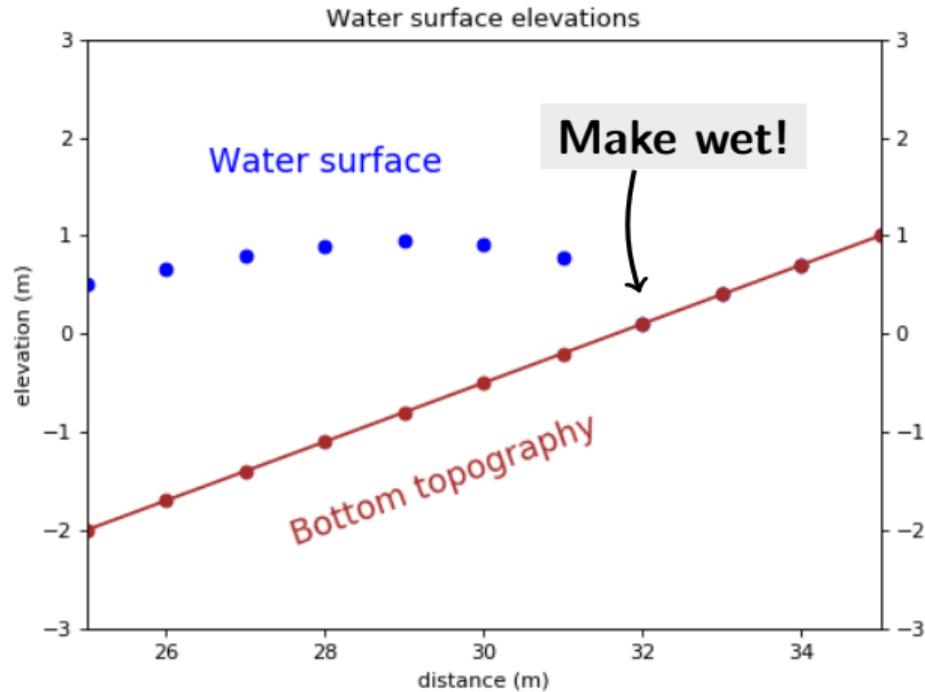
Hybrid theorem proving for verifying numerical software

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Hybrid theorem proving for verifying numerical software

Hybrid theorem proving for verifying numerical software



Hybrid theorem proving for verifying numerical software

Hybrid theorem proving for verifying numerical software

1-D shallow water equations:

$$\eta' = -\frac{\partial uh}{\partial x}, \dots \quad (1)$$

► In an **actual numerical model**, discretize both in time and space:

$$\frac{\eta_i^{n+1} - \eta_i^n}{\Delta t} = \left((uh)_{i+1}^n - (uh)_{i-1}^n \right) / (\Delta x), \dots \quad (2)$$

► In a **hybrid verification model**, discretize in space only:

$$\eta' = \left((uh)_{i+1} - (uh)_{i-1} \right) / (\Delta x), \dots \quad (3)$$

where η is water elevation, h is water height, u is velocity.

Hybrid theorem proving for verifying numerical software

Abstract discrete grids:

- ▶ Small discrete grids for tractability.
- ▶ Non-determinism to represent external states.

Rationale: By the CFL condition, domain of dependence is limited.

Hybrid theorem proving for verifying numerical software

Hybrid model of the 1-D wetting and drying:

initialConditions() →	<i>initial condition</i>
[{	<i>execution begins</i>
{ $\eta' = (uh_{i+1} - uh_{i-1})/(\Delta x), \dots$ }	<i>continuous evolution</i>
wettingDrying();	<i>discrete assignment</i>
}*]	<i>loop or terminate</i>
safetyCondition()	<i>postcondition</i>

where η is water elevation, h is water height, u is velocity.

Hybrid theorem proving for verifying numerical software

Key elements of the abstraction approach:

- ▶ View numerical software as a hybrid system.
- ▶ Model PDEs as continuous in time and discrete in space (as in the method of lines).
- ▶ Incorporate discrete updates.
- ▶ Work with small, discrete grids.

Test Case: The Keymaera X Model of the KPP scheme

Application of hybrid theorem proving in Earth System Modeling

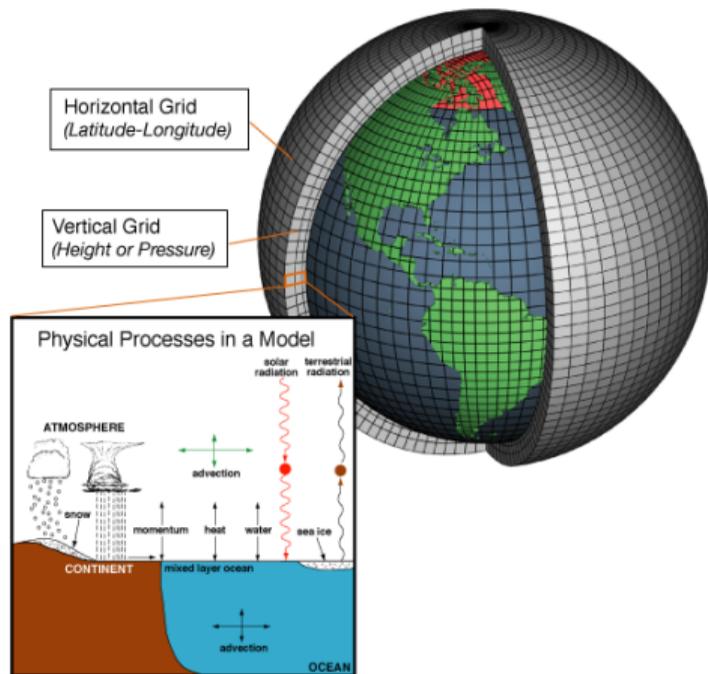
Test Case: The Keymaera X Model of the KPP scheme

- ▶ A test case involving a large-scale numerical software:
 - ▶ **CESM**: A leading climate model developed by NCAR.
 - ▶ **MOM6**: The future ocean component of CESM.
- ▶ **Main Project**: Coupling of MOM6 in CESM
 - ▶ The KPP scheme recently incorporated in MOM6.
 - ▶ An **unphysical behavior** when KPP matching is turned on!

Test Case: The Keymaera X Model of the KPP scheme

Earth System Models:

- ▶ HPC software that simulate Earth's climate.
- ▶ Components: atmosphere, ocean, ice, land, etc.
- ▶ Differential equations that model physical, chemical, and biological processes.
- ▶ Millions of core-hours!



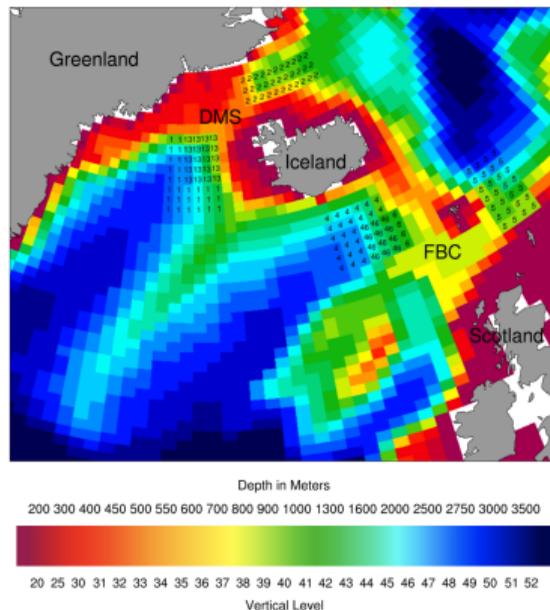
https://celebrating200years.noaa.gov/breakthroughs/climate_model/

Test Case: The Keymaera X Model of the KPP scheme

Horizontal resolution of workhorse ocean grids are $\sim 1^\circ \times 1^\circ$

Global Ocean Models:

- ▶ The 3D primitive equations.
- ▶ Finite difference approximations.
- ▶ Subgrid-scale processes included as parameterizations. Example:
 - ▶ **KPP** scheme parameterizes ocean mixing due to vertical turbulent fluxes in the OBL.



Briegleb et al. (2010, NCAR Tech. Note)

Test Case: The Keymaera X Model of the KPP scheme

The KPP scheme

- ▶ The continuous evolution of a scalar quantity λ over a vertical water column:

$$\frac{\partial \bar{\lambda}}{\partial t} = \frac{\partial}{\partial z} (\overline{w'\lambda'} + \bar{w} \bar{\lambda}) \quad (4)$$

- ▶ The unresolved turbulent flux parameterized as a diffusive process (Griffies et al., 2015):

$$\overline{w'\lambda'} = -K_\lambda \left(\frac{\partial \bar{\lambda}}{\partial z} + \gamma_\lambda \right) \quad (5)$$

- ▶ The diffusivity K_λ at depth d within the OBL (Large et al., 1994):

$$K_\lambda = h \cdot w_\lambda(\sigma) \cdot G_\lambda(\sigma) \quad (6)$$

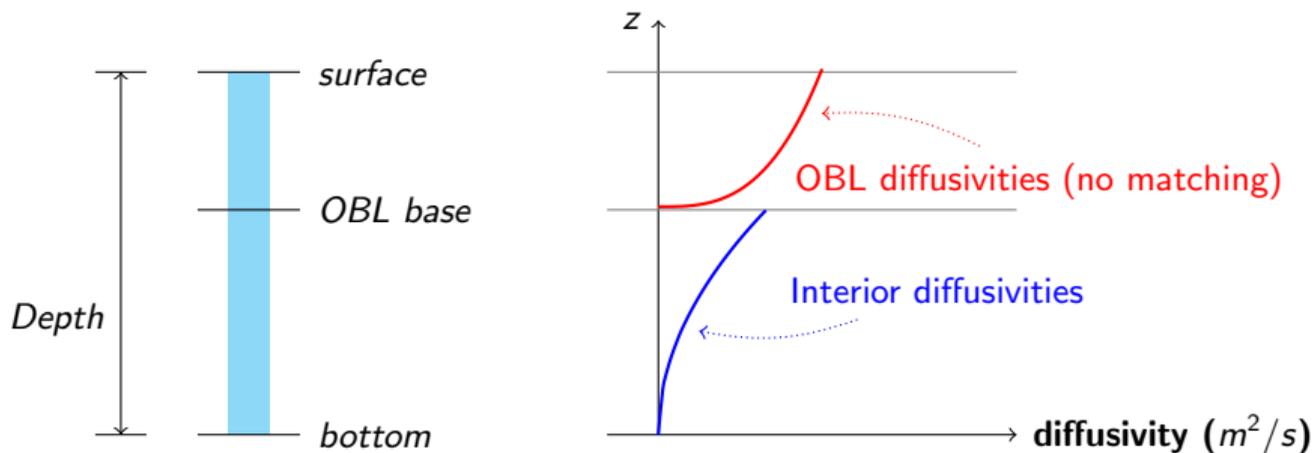
- ▶ Shape function for the OBL diffusivities:

$$G_\lambda(\sigma) = a_0 + a_1\sigma + a_2\sigma^2 + a_3\sigma^3 \quad (7)$$

Test Case: The Keymaera X Model of the KPP scheme

The KPP scheme

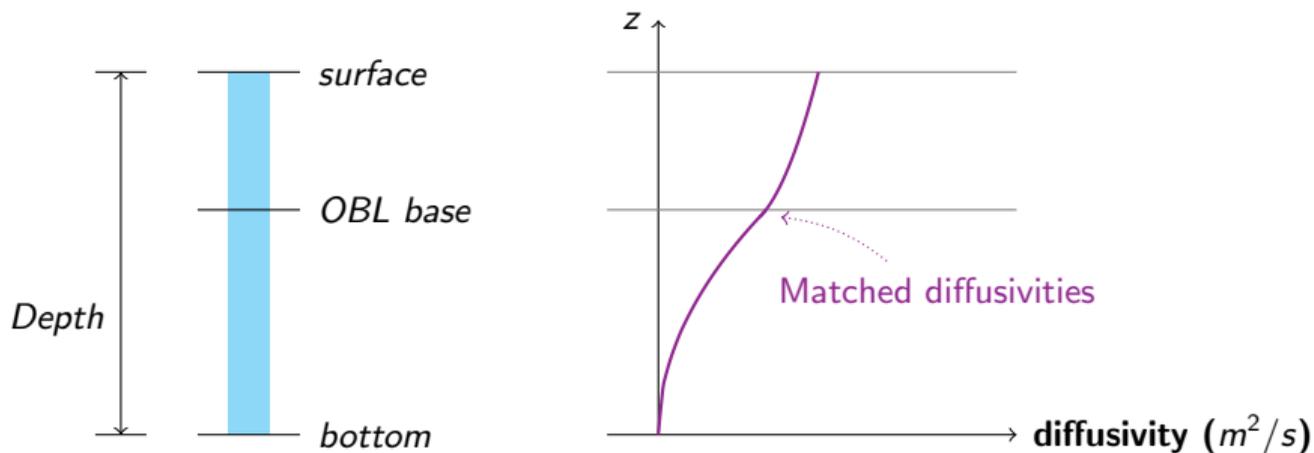
- ▶ Compute the ocean boundary layer (OBL) depth.
- ▶ Compute the diffusivities within ocean interior.
- ▶ Compute the OBL diffusivities (no matching).



Test Case: The Keymaera X Model of the KPP scheme

The KPP scheme

- ▶ Compute the ocean boundary layer (OBL) depth.
- ▶ Compute the diffusivities within ocean interior.
- ▶ Compute the OBL diffusivities (**matching**).



Test Case: The Keymaera X Model of the KPP scheme

- ▶ **Undesired behavior:**
 - ▶ Matching algorithm leads to negative diffusivities in OBL.
- ▶ **Debugging:**
 - ▶ Via an interactive debugger.
 - ▶ Took several days and thousands of CPU hours.
- ▶ **Fix:**
 - ▶ Modify the matching algorithm for cases where the interior diffusivity gradient is negative.
- ▶ **Verification:**
 - ▶ A KeYmaera X model of the KPP scheme.

Test Case: The Keymaera X Model of the KPP scheme

The hybrid model of the KPP scheme:

	<i>initialConditions()</i> →	
timestep	{	<i>compute_OBL_depth;</i> // <i>discrete updates</i>
		<i>compute_interior_K;</i>
		<i>compute_OBL_K;</i>
		{ <i>z'_{cr} = -z_{cr}</i> } // <i>continuous system</i>
		}*
		<i>K > 0</i>

where K is diffusivity and z_{cr} is the depth at which Ri_B is equal to Ri_{cr} .

Test Case: The Keymaera X Model of the KPP scheme

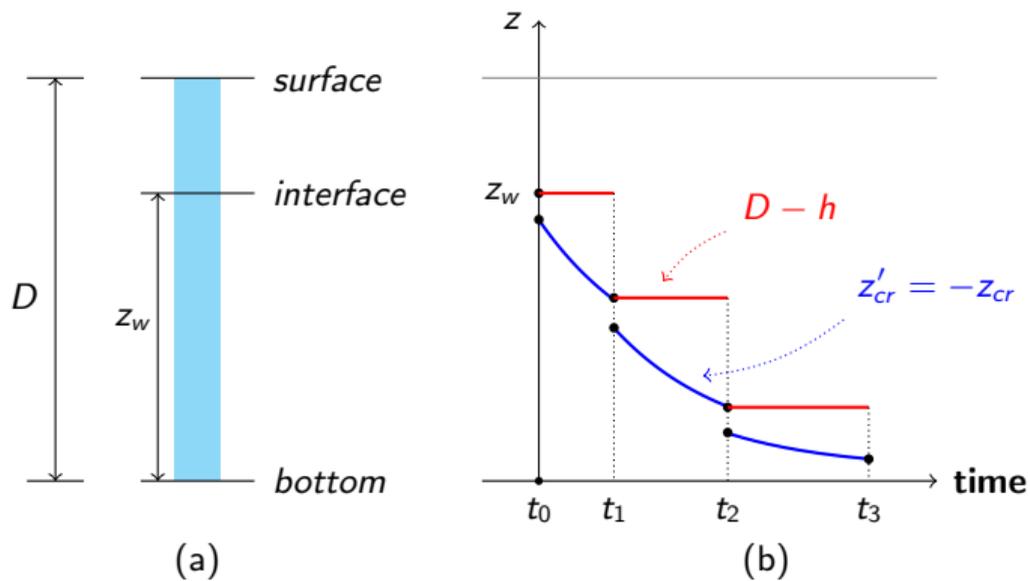
The hybrid model of the KPP scheme:

	<i>initialConditions()</i> →	
	[{	
instantaneous	{	<i>compute_OBL_depth;</i> // <i>discrete updates</i>
	{	<i>compute_interior_K;</i>
	{	<i>compute_OBL_K;</i>
over some Δt	{	{ $z'_{cr} = -z_{cr}$ } // <i>continuous system</i>
	{*]	
	$K > 0$	

where K is diffusivity and z_{cr} is the depth at which Ri_B is equal to Ri_{cr} .

Test Case: The Keymaera X Model of the KPP scheme

Continuous evolution of z_{cr} + discrete changes:

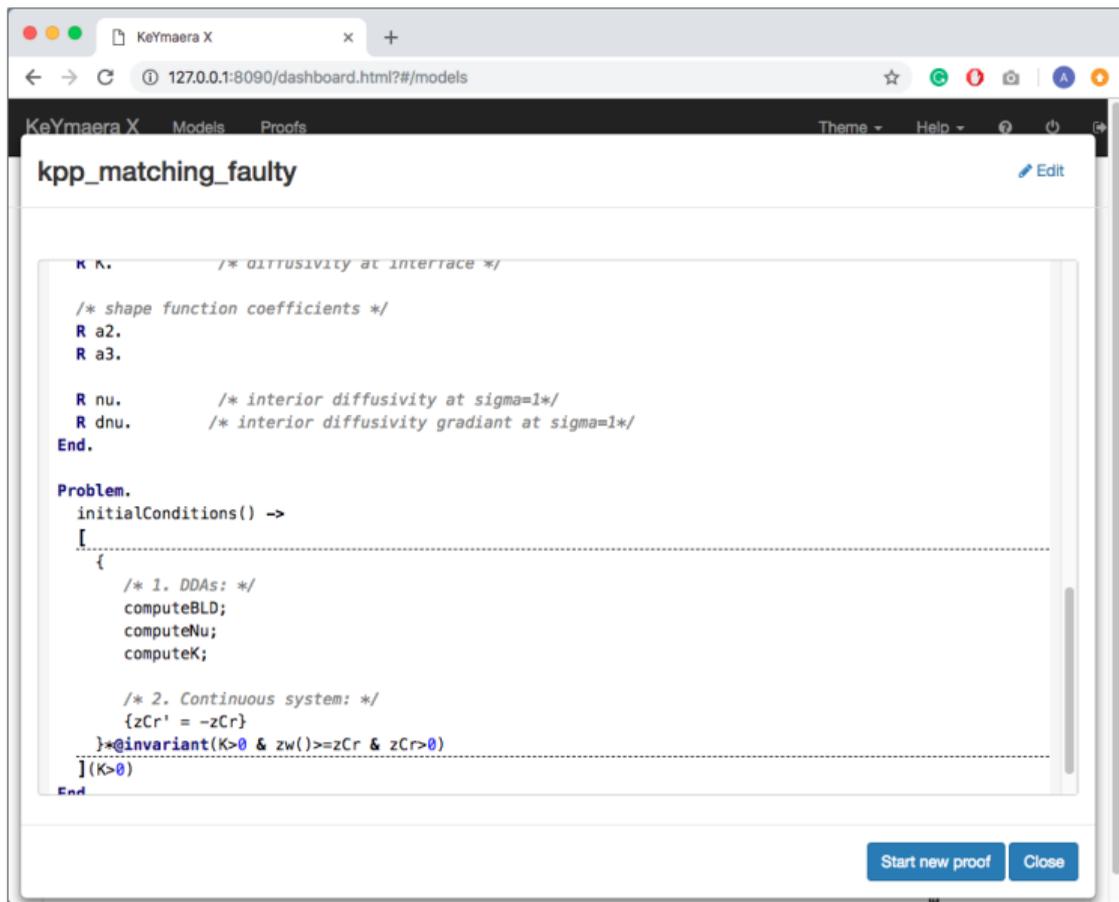


Test Case: The Keymaera X Model of the KPP scheme

The KeYmaera X proof process:

1. Develop the hybrid model of the KPP scheme
2. Reproduce the undesired behavior via a custom proof tactic:
 - ▶ Conventional logical assertions and rules, e.g.,
 - ▶ loop invariants
 - ▶ as well as *differential dynamic logic* rules, e.g.,
 - ▶ differential invariants
3. Apply the fix in the matching algorithm: match gradients only if interiorgradients are non-negative.
4. Re-run the proof tactic and confirm that undesired behavior is eliminated.

KeYmaera X UI:
Develop the hybrid model.



KeYmaera X UI: Construct a proof.

The screenshot shows the KeYmaera X web interface. The browser address bar displays the URL `127.0.0.1:8090/dashboard.html?#/proofs/109`. The page title is "KeYmaera X" and the navigation menu includes "Models" and "Proofs". The main content area is titled "kpp_matching_faulty: Proof 3". Below the title, there is a toolbar with buttons for "Auto", "Unfold", "Prop-Auto", "Simplify", "Step back", "Edit", and "Browse...". A dropdown menu is open, showing options: "Propositional", "Quantifiers", "Hybrid Programs", "Differential Equations", "Closing", and "Inspect". The main proof area displays a goal:
$$\vdash D > 0 \wedge D > zw \wedge zw > 0 \wedge 0 < nu \wedge K > 0 \wedge w > 0 \wedge zCr = zw \rightarrow [\{ \{ h := D - zCr ; \sigma := (D - zw) / h ; \alpha := * ; ? 0 < \alpha \wedge \alpha < 1 ; zCr := \alpha * zCr ; \} \{ nu := * ; ? nu > 0 ; dnu := * ; \} \{ a2 := -2 + 3 * nu / (h * w) + dnu / w ; a3 := 1 - nu / (h * w) - dnu / w ; K := h * w * (\sigma + a2 * \sigma^2 + a3 * \sigma^3) ; \} \{ zCr' = -zCr \ \& \ true \}] * K > 0$$
 A hint "(MPLVR)" is visible to the right of the goal. Below the goal, there is a "Proof Progra..." section with buttons for "Rerun", "Fresh steps", "None", "Execute:", "Atomic", and "Step-by-Step". The current state of the proof is "nil". The footer of the interface reads: "KeYmaera X version 4.4.3 (version 4.6.1 is now available from KeYmaeraX.org). © Logical Systems Lab, Carnegie Mellon University 2017".

KeYmaera X UI: Steer the proof.

The screenshot shows the KeYmaera X web interface. At the top, the browser address bar displays the URL `127.0.0.1:8090/dashboard.html?#/proofs/109`. The interface includes a navigation bar with "Models" and "Proofs" tabs, and a toolbar with buttons for "Auto", "Unfold", "Prop-Auto", "Simplify", "Step back", "Edit", and "Browse...". Below the toolbar, there are dropdown menus for "Propositional", "Quantifiers", "Hybrid Programs", "Differential Equations", "Closing", and "Inspect".

The main area displays a proof goal:

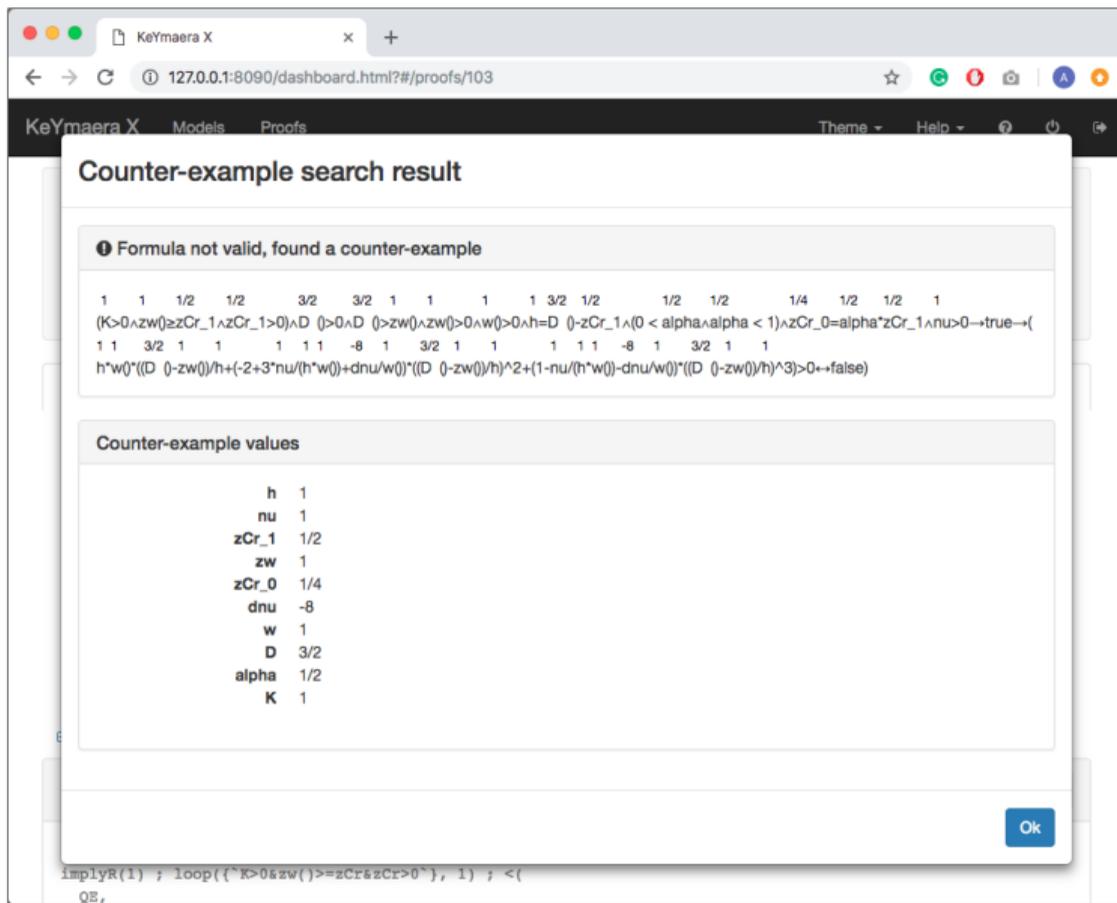
$$\vdash D > 0 \wedge D > zw \wedge zw > 0 \wedge 0 < nu \wedge K > 0 \wedge w > 0 \wedge zCr = zw \rightarrow [\{ \{ h := D - zCr ; \sigma := (D - zw)/h ; \alpha := * ; ? 0 < \alpha \wedge \alpha < 1 ; zCr := \alpha * zCr ; \} \{ nu := * ; ? nu > 0 ; dnu := * ; \} \{ a2 := -2 + 3 * nu / (h * w) + dnu / w ; a3 := 1 - nu / (h * w) - dnu / w ; K := h * w * (\sigma + a2 * \sigma^2 + a3 * \sigma^3) ; \} \{ zCr' = -zCr \ \& \ true \}] * K > 0$$

A "Loop Induction" lemma dialog is open, showing a proof structure:

$$\frac{\Gamma \vdash K > 0 \wedge zw() \geq z \dots, \Delta \quad \frac{K > 0 \wedge zw() \geq z \dots \quad K > 0 \wedge zw() \geq z \dots}{\vdash P}}{\Gamma \vdash [a^*]P, \Delta}$$

The dialog also includes a search bar for lemmas and buttons for "Browse..." and "Apply Lemma".

KeYmaera X UI:
 Generate counter-example
 if formula is invalid.



KeYmaera X UI:
Close the proof.

KeYmaera X

127.0.0.1:8090/dashboard.html?#/proofs/97

Proof Result

✓ All goals in your proof agenda have been closed.

Provable

```
NoProofTermProvable(Provable( ==> D()>0&D()>zw()&zw()>0&0 < nu&K>0&w()>0&zCr=zw()->[{{h:=D()-zCr;sigma:=D()-zw()/h;alpha:=*;?0 < alpha&alpha < 1;zCr:=alpha*zCr;}{nu:=*;?nu>0;dnu:=*};{?dnu < 0;a2:=-2+3*nu/(h*w());a3:=1-nu/(h*w());++?dnu>=0;a2:=-2+3*nu/(h*w())+dnu/w();a3:=1-nu/(h*w())-dnu/w();}K:=h*w()*(sigma+a2*sigma^2+a3*sigma^3);}{zCr'=-zCr&true}*}K>0 proved))
```

Tactic to Reproduce the Proof

```
implyR(1) ; loop({'K>0&zw()>=zCr&zCr>0'}, 1) ; <(
  QE,
  QE,
  composeb(1) ; composeb(1) ; assignb(1) ; composeb(1) ; assignb(1) ; composeb(1) ; randomb(1) ; a
  llR(1) ; composeb(1) ; testb(1) ; implyR(1) ; assignb(1) ; composeb(1) ; composeb(1) ; randomb(1)
  ; allR(1) ; composeb(1) ; testb(1) ; implyR(1) ; randomb(1) ; allR(1) ; composeb(1) ; composeb(1)
  ; choiceb(1) ; composeb(1.0) ; testb(1.0) ; andR(1) ; <(
    implyR(1) ; composeb(1) ; assignb(1) ; assignb(1) ; assignb(1) ; boxAnd(1) ; andR(1) ; <(
      dW(1) : trueTmlv(1) : 0F.
```

KeY

[Browse proof](#) [Download tactic](#) [Download lemma](#) [Download archive](#) [Close](#)

Conclusions

- ▶ A lightweight formal methods application.
- ▶ Highly efficient compared to testing.
- ▶ Provides more confidence.
 - ▶ Generality (due to nondeterminism)
 - ▶ The coverage in the temporal dimension is much greater.
- ▶ Limitations:
 - ▶ floating point arithmetic
 - ▶ numerical issues

Thanks

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