

visualCaseGen Streamlining CESM Simpler Modeling Efforts and Beyond

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Goals:

- Streamline CESM simpler modeling efforts and beyond.
- Enable hierarchical modeling: explore/combine different complexity levels.

In Practical Terms:

- Browse existing CESM configurations efficiently.
- Quickly generate new configurations (compsets and grids):
 - Mix and match models and settings in a compatible manner.
 - Create or modify grids as needed.



Part 1: A quick tour of visualCaseGen:

A GUI that guides the user through the process of creating experiments.



visualCaseGen

visualCaseGen

Welcome to visualCaseGen!

visualCaseGen guides users through the process of creating CESM experiments.

Start

Click to add a cell.

? Help

1

Part 2: A Glimpse Inside visualCaseGen Software



visualCaseGen

How Does visualCaseGen Determine Compatibility?

- Constraint Specification: Defines relationships between config variables.
- Constraint Solver: Utilizes the Z3 library for logical reasoning.



The Z3 Library

What it Does: Checks if a set of constraints can be satisfied. Finds solutions.

Strengths: Combines logical reasoning with knowledge about specific domains (bools, ints, reals, strings, etc.). Manages complex relationships.

Development and Usage:

- Widely used in academia and industry. (~10k Citations, ~10k GitHub Stars)
- Developed by Microsoft Research. Open source and free (MIT license).
- Robust Python API. Available via pip.



Relational Constraint Specification in visualCaseGen



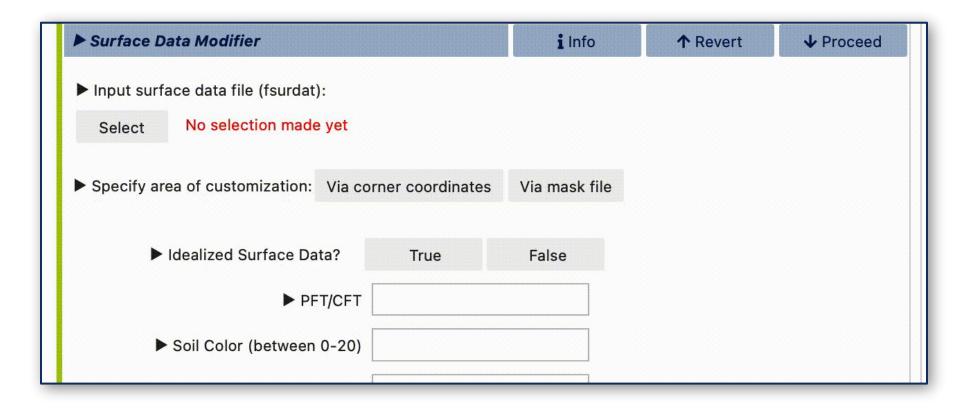
LND_DOM_PFT >= 0.0:

"PFT/CFT must be set to a nonnegative number"



$LND_DOM_PFT >= 0.0:$

"PFT/CFT must be set to a nonnegative number"





Or(COMP_OCN=="mom", OCN_GRID_MODE=="Standard"):

"Custom OCN grids can only be generated for MOM6."



Or(COMP_OCN=="mom", OCN_GRID_MODE=="Standard"):
 "Custom OCN grids can only be generated for MOM6."

► Components			i Info	C ^e Reset	↑ Revert	↓ Proceed
▼ ATM	▼ LND	▼ ICE	▼ OCN	▼ ROF	▼ GLC	▼ WAV
datm	clm	cice5	рор	rtm	cism	🗙 ww3
🗙 satm	slim	cice	mom	mosart	dglc	ww3dev
cam	dInd	dice	docn	mizuroute	sglc	dwav
	sInd	sice	socn	drof		swav
				srof		



Or(COMP_OCN=="mom", OCN_GRID_MODE=="Standard"):
 "Custom OCN grids can only be generated for MOM6."

► Components			i Info	C'Reset	↑ Revert	↓ Proceed
▼ ATM	▼ LND	▼ ICE	▼ OCN	▼ ROF	▼ GLC	▼ WAV
datm	clm	cice5	рор	rtm	cism	🗙 ww3
🗙 satm	slim	cice	mom	mosart	dglc	ww3dev
cam	dInd	dice	docn	mizuroute	sglc	dwav
	sInd	sice	socn	drof		swav
				srof		
► Ocean Grid Mode			i Info	C'Reset	↑ Revert	↓ Proceed
Ocean Grid Mode: Standard 🗙			🗙 Create New			



Implies(And(COMP_OCN=="mom", COMP_LND=="slnd", COMP_ICE=="sice"), OCN_LENY<180.0):
 "If LND and ICE are stub, custom MOM6 grid must exclude poles (singularity).",</pre>



The constraint specification syntax might seem unfamiliar at first.

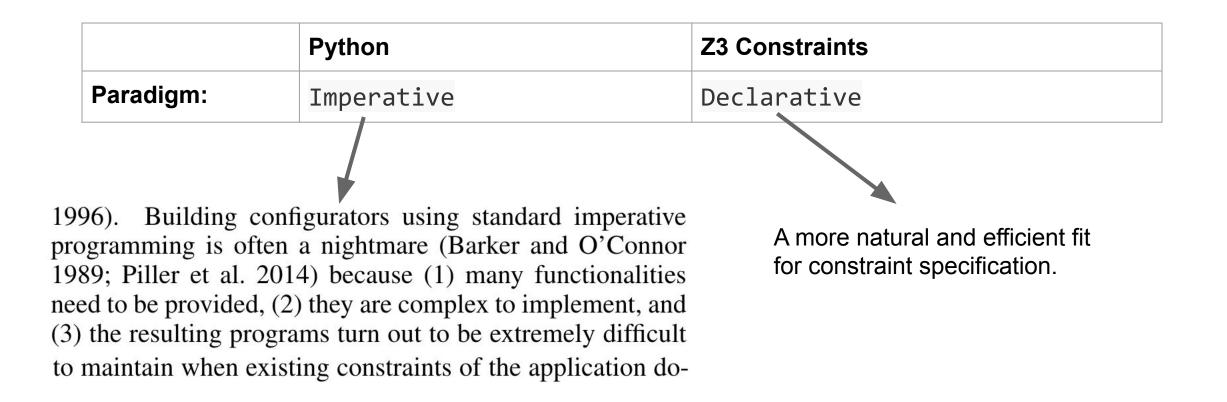


	Python	Z3 Constraints
Comparison	==, !=, >, <, >=, <=	same
Arithmetic	+, -, *, /	same
Logical	p and q p or q not p not p or q	And(p, q) Or(p, q) Not(p) Implies(p, q)
String	a in b a.startswith(b) 	Contains(b, a) PrefixOf(a,b)



	Python	Z3 Constraints
Paradigm:	Imperative	Declarative





Carbonnelle, Pierre, et al. "Interactive configurator with FO (.) and IDP-Z3." (2022).



The constraint specification syntax might seem unfamiliar at first, *but* it enables the use of z3 as the core of the visualCaseGen constraint solver.



Why use a solver?

Constraint satisfaction problem (CSP) is inherently complex (NP-complete).

- **Hidden Conflicts**: Individual constraints might be satisfied, but their combinations can lead to conflicts.
- **Dead-Ends:** Solvers prevent scenarios where no feasible options remain for configuration variables.
- **Constraint Analysis**: Are the constraints satisfiable? Any unreachable options? Any constraint redundant?
- **Scalability and Efficiency:** As variables and constraints increase, complexity grows exponentially. CSP solvers tackle this efficiently.



Implies(COMP_WAV=="ww3", In(COMP_OCN, ["mom", "pop"])):
 "WW3 can only be selected if either POP2 or MOM6 is the ocean component.",

Implies(COMP_ATM=="satm", COMP_OCN=="socn"):

"An active/data atmosphere is needed to force the ocean model."



Implies(COMP_WAV=="ww3", In(COMP_OCN, ["mom", "pop"])):
 "WW3 can only be selected if either POP2 or MOM6 is the ocean component.",

Implies(COMP_ATM=="satm", COMP_OCN=="socn"):

"An active/data atmosphere is needed to force the ocean model."

Components				i Info	↑ Revert	↓ Proceed
▼ ATM	▼ LND	▼ ICE	▼ OCN	▼ ROF	▼ GLC	▼ WAV
datm	clm	cice5	рор	rtm	cism	ww3
satm	slim	cice	mom	mosart	dglc	ww3dev
cam	dInd	dice	docn	mizuroute	sglc	dwav
	sInd	sice	socn	drof		swav
				srof		



```
Implies(COMP_LND=="clm", COMP_ROF!="drof") :
    "CLM cannot be coupled with a data runoff model.",
Implies(COMP_LND=="slim", And(COMP_GLC=="sglc", COMP_ROF=="srof", COMP_WAV=="swav")) :
    "GLC, ROF, and WAV cannot be coupled with SLIM.",
Implies(COMP_OCN=="mom", COMP_WAV!="dwav") :
    "MOM6 cannot be coupled with data wave component.",
Implies(COMP_LND=="slnd", Or(COMP_OCN=="mom", COMP_GLC=="sglc")) :
    "GLC cannot be coupled with a stub land model, unless it is coupled with MOM6.",
Implies(COMP_LND=="dlnd", COMP_ATM!="cam"):
    "CAM-DLND coupling is not supported.",
```



```
Implies(COMP_LND=="clm", COMP_ROF!="drof") :
    "CLM cannot be coupled with a data runoff model.",
Implies(COMP_LND=="slim", And(COMP_GLC=="sglc", COMP_ROF=="srof", COMP_WAV=="swav")) :
    "GLC, ROF, and WAV cannot be coupled with SLIM.",
Implies(COMP_OCN=="mom", COMP_WAV!="dwav") :
    "MOM6 cannot be coupled with data wave component.",
```

Implies(COMP_LND=="slnd", Or(COMP_OCN=="mom", COMP_GLC=="sglc")) :

Components				i Info	↑ Revert	↓ Proceed
▼ ATM	▼ LND	▼ ICE	▼ OCN	▼ ROF	▼ GLC	▼ WAV
datm	clm	cice5	рор	rtm	cism	ww3
satm	slim	cice	mom	mosart	sglc	ww3dev
cam 🔐	dInd	dice	docn	mizuroute		dwav
	sInd	sice	socn	drof		swav
				srof		



The bottom line,

The interaction of constraints, even simple ones, can lead to hidden conflicts, dead ends, and chain reactions. Robust constraint handling is vital.



The **Stage** Concept in visualCaseGen and some key lessons in <u>software design</u>



Stage: A collection of config variables that can be configured simultaneously.

Frontend Representation:

► Components				i Info	↑ Revert	↓ Proceed
▼ ATM	▼ LND	▼ ICE	▼ OCN	▼ ROF	▼ GLC	▼ WAV
datm	clm	cice5	рор	rtm	cism	ww3
satm	slim	cice	mom	mosart	dglc	ww3dev
cam	dInd	dice	docn	drof	sglc	dwav
	sInd	sice	socn	srof		swav



Stage is a *hierarchical* concept.

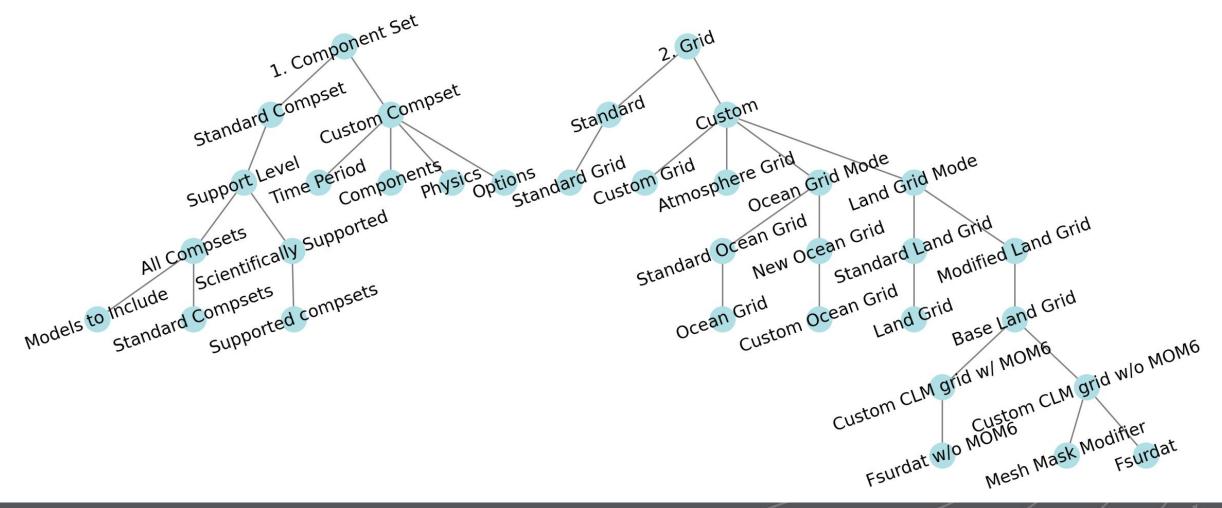
parent	1. Component Set						
` (Configuration Mode:	Standard	Custom				
	► Time Period			i Info	↑ Revert	↓ Proceed	Siblings
	Initialization Time:	1850	2000	HIST			1.95
	-						
	Components						
	Component Physics						

• Based on the hierarchy, visualCaseGen generates a Stage tree and pipeline.



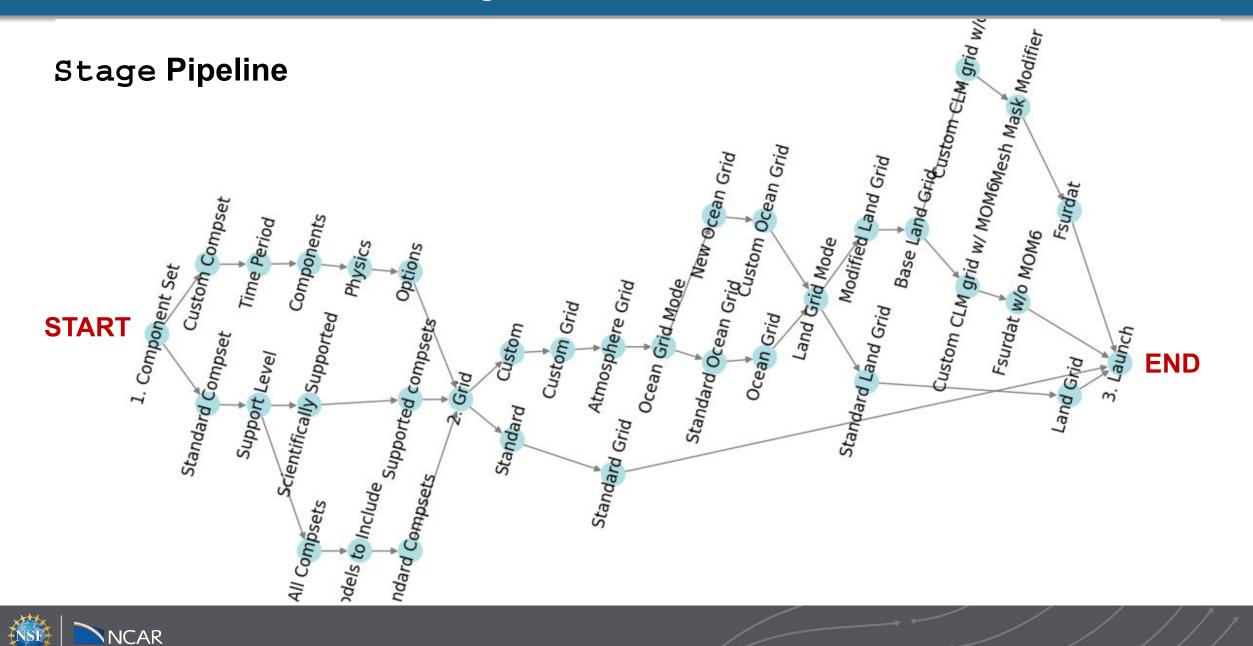
The Stage Concept in visualCaseGen

Stage Tree

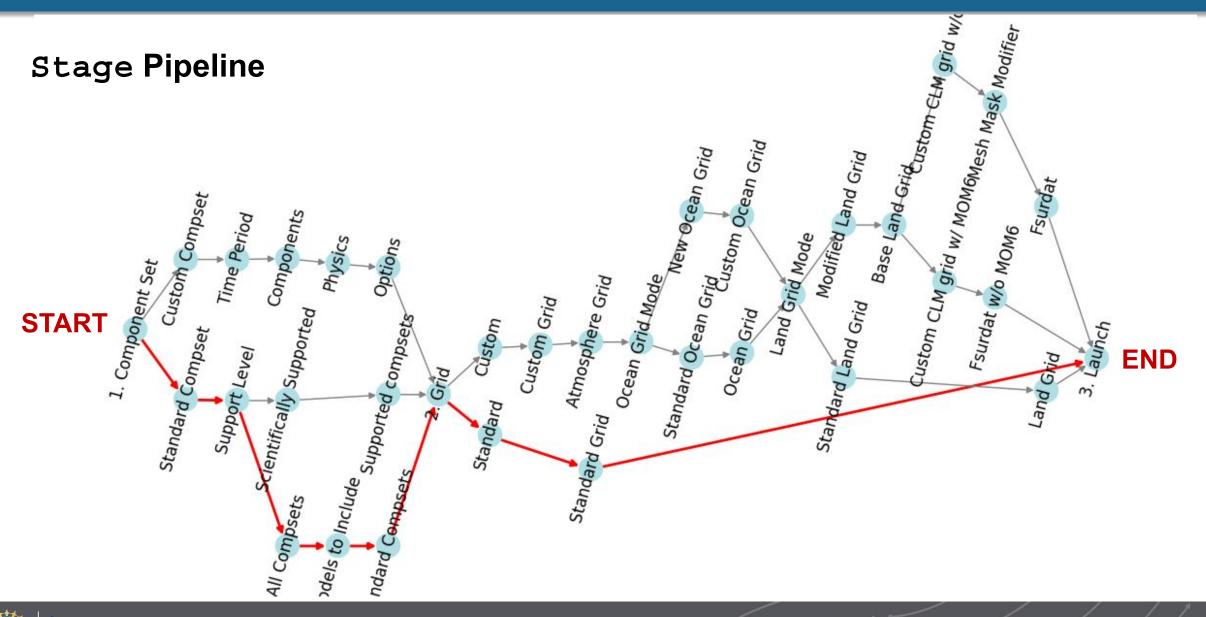




The Stage Concept in visualCaseGen



The Stage Concept in visualCaseGen





Stage pipeline dictates *variable precedence*, such that:

- Variables in earlier stages have higher precedence.
- Variables within the same stage have equal precedence.

A complicating factor: The same variable can appear in multiple stages, as long as they are not reachable along the same path.



The Stage Pipeline must form a directed acyclic graph (DAG). This ensures that:

- A consistent variable precedence can be established.
- No cycles are encountered by the user.



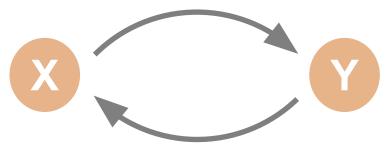
Stage Mechanism + Constraint Solver



Constraint Graph: Formed by the specified constraints and variable precedence.

• For each variable **X** and **Y** occurring in the same constraint:

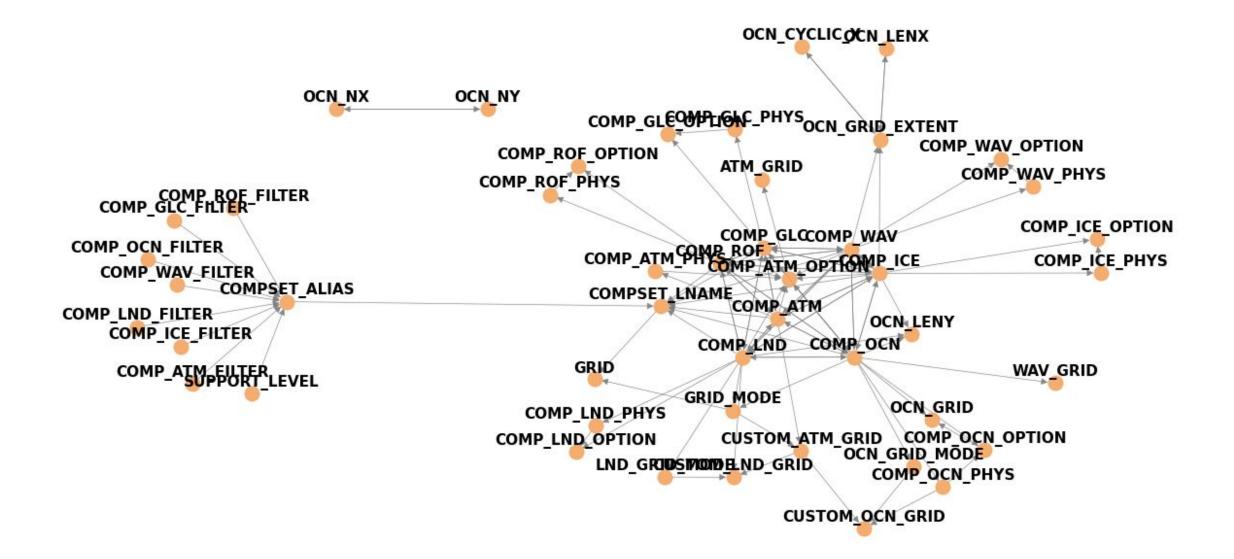
 $Precedence(X) \ge Precedence(Y)$



 $Precedence(X) \leq Precedence(Y)$



Constraint Graph

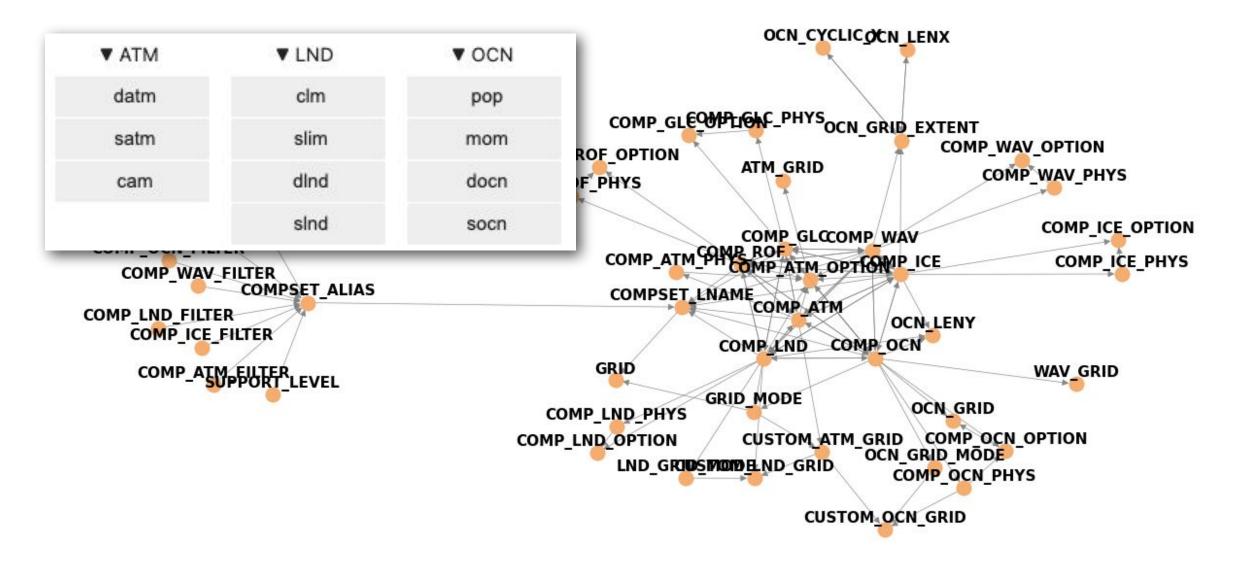




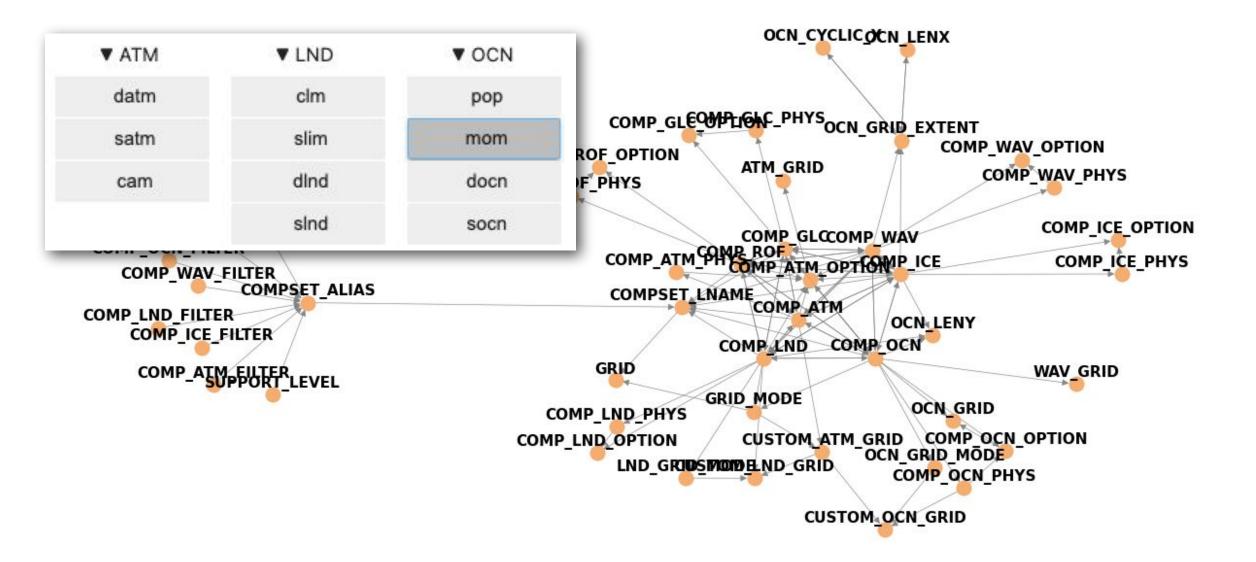
A user change initiates a traversal of the constraint graph:

- All potentially affected variables are visited: This involves calling Z3 to check if the validity of options changed.
- The extent of the traversal depends on the user input, the stage hierarchy, and constraints.

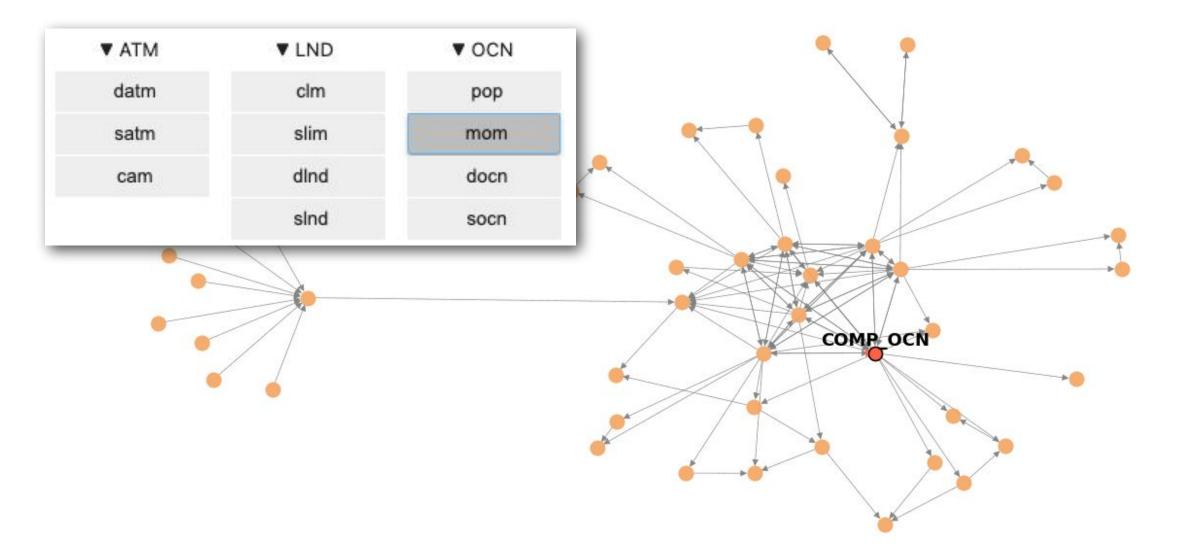




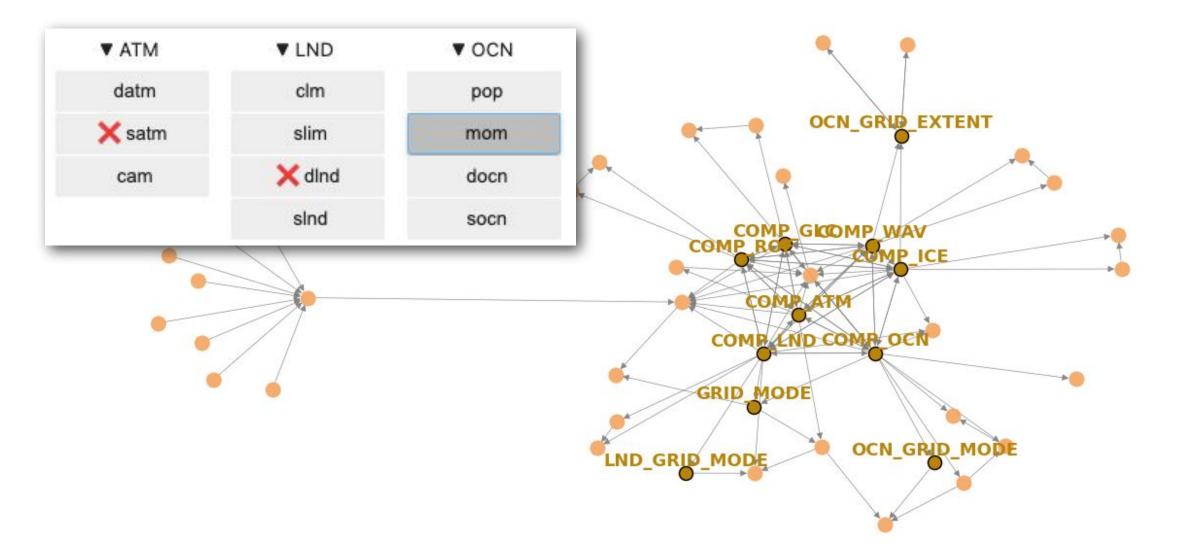














Conceptual Construct Matters.



Prototype vs Product

visualCaseGen	- Custom Mod	e			🕱 Help	් Reset
Initialization Time:	:					
1850	2000	HIST				
Components:						
▼ ATM	▼ LND	▼ ICE	▼ OCN	▼ ROF	▼ GLC	▼ WAV
datm	clm	cice5	рор	rtm	cism	ww3
satm	slim	cice	mom	mosart	dglc	ww3dev
cam	dInd	dice	docn	mizuroute	sglc	dwav
	sInd	sice	socn	drof		swav
				srof		
Physics and Opti	ions:					
АТМ	LND	ICE	OCN	ROF	GLC	WAV
Options will be o	lisplayed here afte	er a component sel	ection.	compset: not	all component phy	/sics selected ye
		Grid Selection Mo	de: Predefined	Custom		

Standard Cust 1850 2	om 2000 HIST			
1850 2	000			
1850 2	0000			
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▼ ICE	▼ OCN	▼ ROF	▼ GLC	▼ WAV
cice5	рор	rtm	cism	ww3
cice	mom	mosart	dglc	ww3dev
dice	docn	mizuroute	sglc	dwav
sice	socn	drof		swav
		srof		
,	cice5 cice dice	cice5 pop cice mom dice docn	▼ICE ▼OCN ▼ROF Cice5 pop rtm Cice mom mosart dice docn mizuroute sice socn drof	▼ICE ▼OCN ▼ROF ▼GLC Cice5 pop rtm cism Cice mom mosart dglc dice docn mizuroute sglc sice socn drof



With the introduction of the **Stage** Concept:

- **UX enhanced**: Clearer guidance on user actions.
- **Robustness increased**: Clearer requirements and invariants such as variable precedence, state change rules, and relational dependencies.
- Maintainability improved: LOC decreased significantly.
- **Better performance**: A more efficient constraint solver implementation tripled the computational performance.



Software architecture is infrequently discussed or considered: Focus tends to be on low-level details.

But high-level design constructs (i.e., functionalities, patterns, structures) have a significant influence on overall software quality. We should make sure:

- All the conceptual constructs are identified, incorporated, and documented.
- The relationships between them are well-established and understood.
- Requirements are carefully analyzed and adhered to.



The hard part of building software is the conceptual construct, not the labor of representing it.

- FP Brooks. "No Silver Bullet" (1987)



The hard part of building software is the conceptual construct, not the labor of representing it.

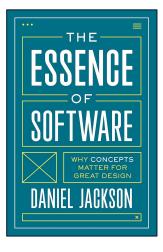
- FP Brooks. "No Silver Bullet" (1987)

Agilistas prioritize **code** over **design + requirements + specifications**. But in 10 years, those will be the only things we'll write.

- Daniel Jackson, "What Makes Software Work?" (2024)



References

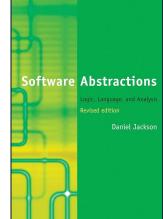


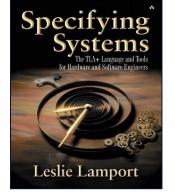
"What matters is the fundamental structure of the design. If you get it wrong, there is no amount of bug fixing and refactoring that will produce a reliable, maintainable, and usable system."

- D. Jackson. The essence of software. (2021)

"Code is a poor medium for exploring abstractions."

– D. Jackson. Software Abstractions. (2012)

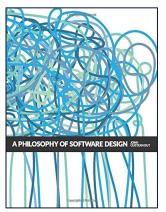




"Writing is nature's way of letting you know how sloppy your thinking is." – L. Lamport. *Specifying Systems*. (2002)

"Be on the lookout for opportunities to improve the design and plan on spending some fraction of your time on design improvements."

– J. Ousterhout. *A Philosophy of Software Design*. (2018)





A stable beta version released and available at: https://github.com/ESMCI/visualCaseGen

Official release this winter.

Thanks!

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