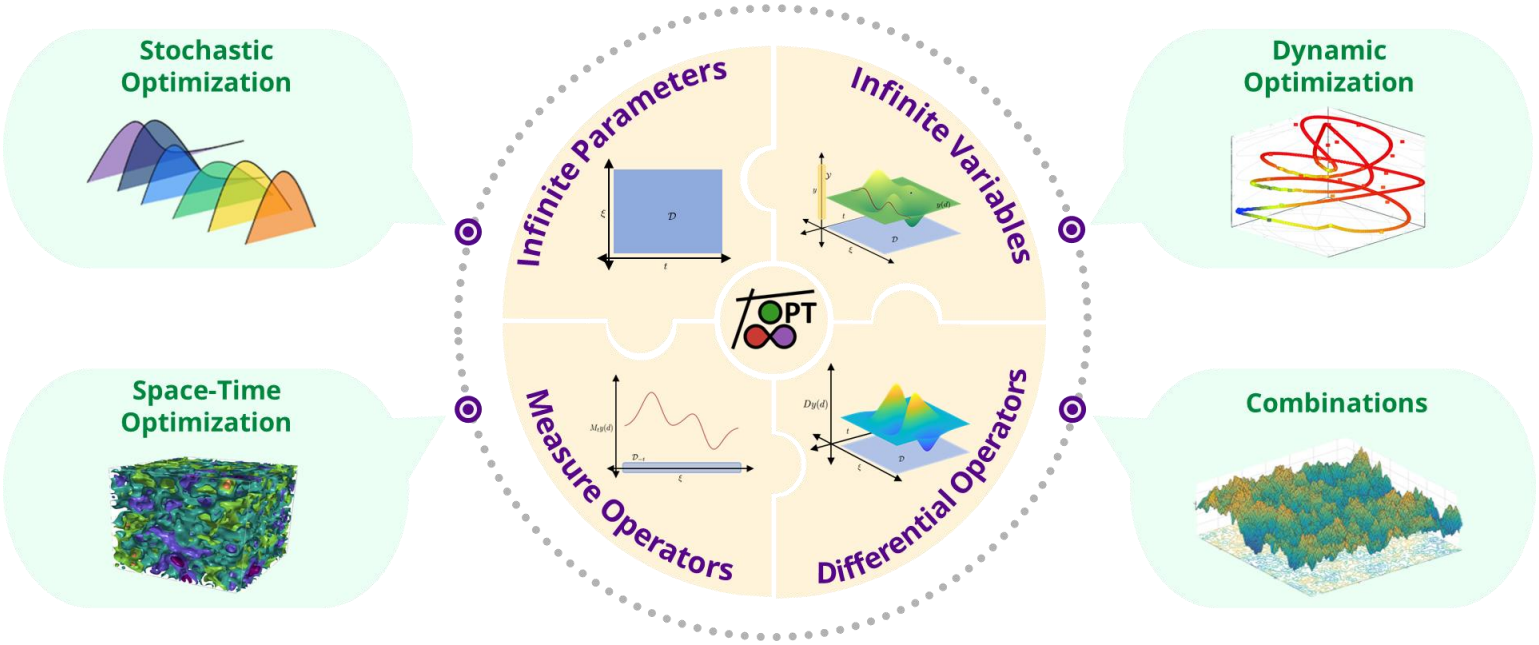
THE STATE OF InfiniteOpt

Joshua Pulsipher



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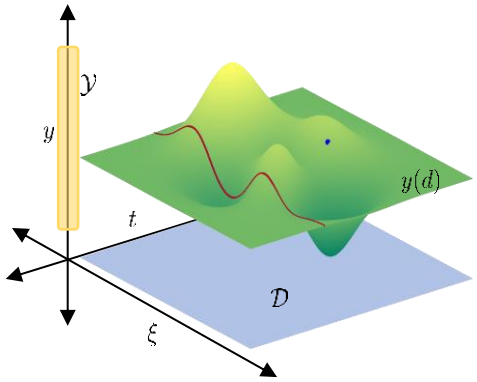
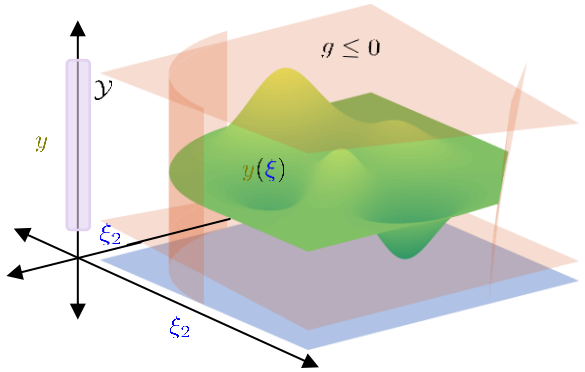
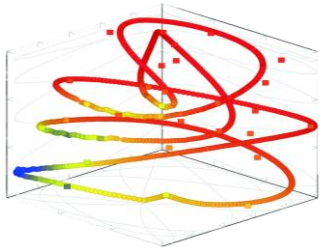
WHAT IS INFINITE-DIMENSIONAL OPTIMIZATION?

- Variables and/or constraints **indexed over continuous domains**

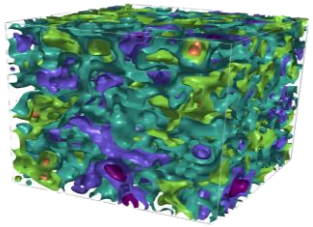




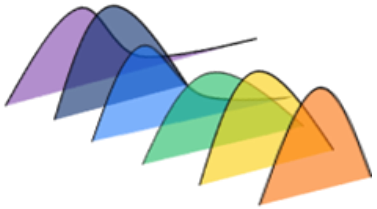
- Three common domains



Time



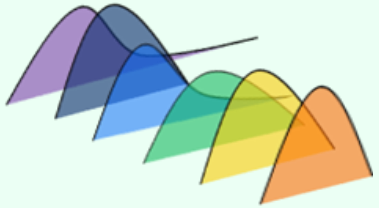
Space



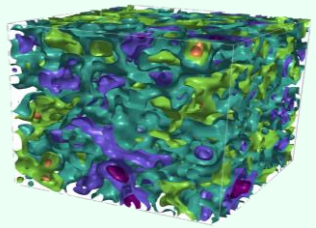
Uncertainty

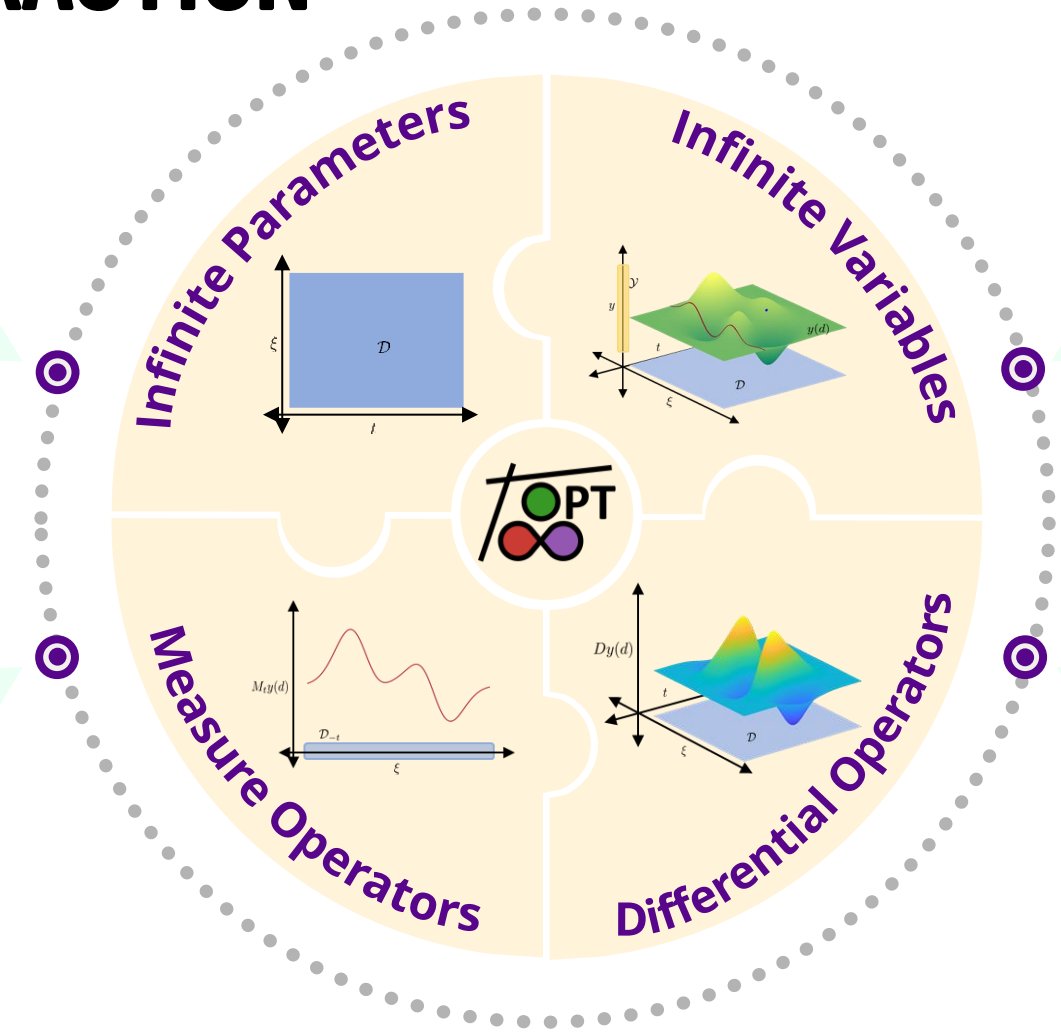
UNIFYING ABSTRACTION

Stochastic Optimization

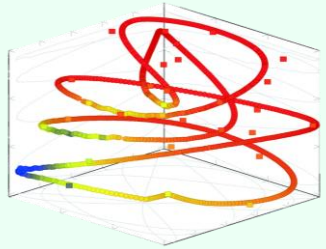


Space-Time Optimization

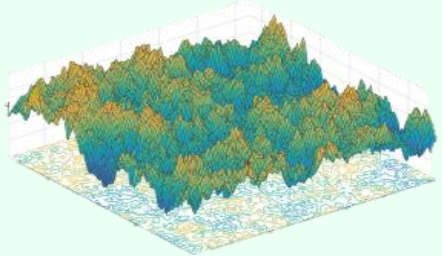




Dynamic Optimization



Combinations



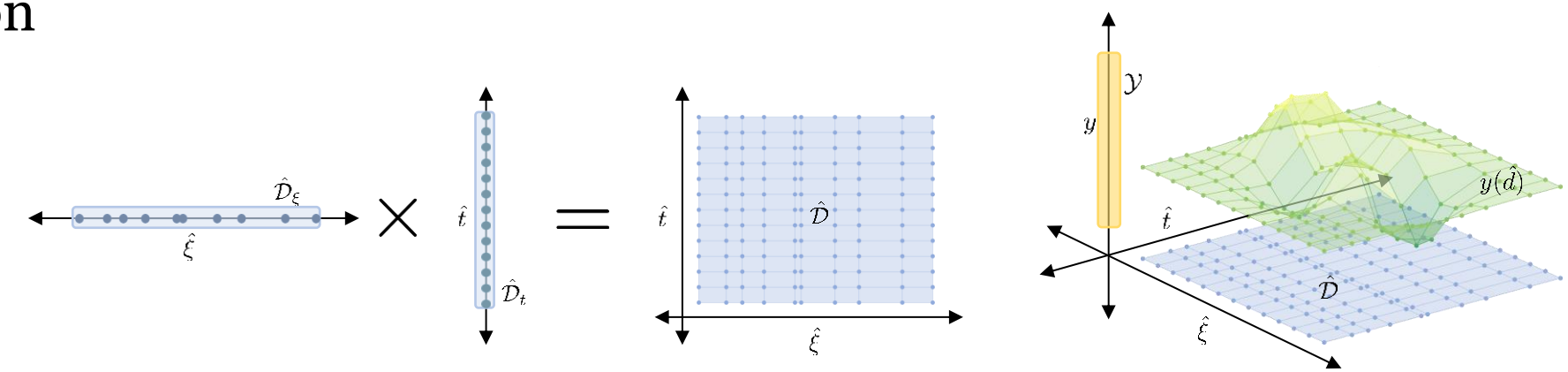
J. L. Pulsipher, W. Zhang, T. J. Hongisto, and V. M. Zavala. "A unifying modeling abstraction for infinite-dimensional optimization." 2022

SOLUTION VIA TRANSFORMATION

- Direct Transcription

Project onto set of **finite points** $\hat{\mathcal{D}}$

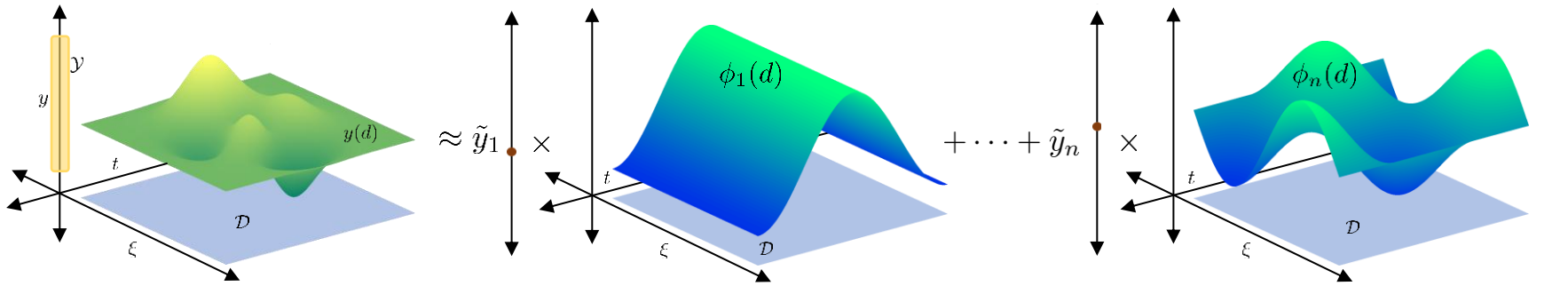
$$\hat{\mathcal{D}} := \prod_{\ell \in \mathcal{L}} \{\hat{d}_{\ell,i} : \hat{d}_{\ell,i} \in \mathcal{D}_\ell, i \in \mathcal{I}_\ell\}$$



- Alternative Methods

Project onto set of known **basis functions**

$$y(d) \approx \sum_{i \in \mathcal{I}} \tilde{y}_i \phi_i(d)$$

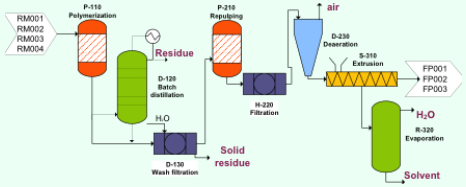


APPLICATIONS

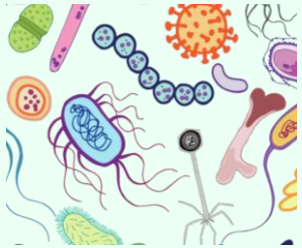
Unifying Abstraction

Dynamic Optimization
(Time)

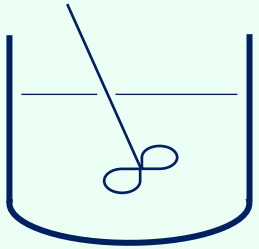
Autonomous Vehicles



Process Control

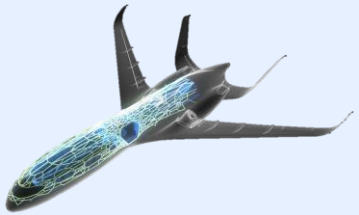


Bioprocessing

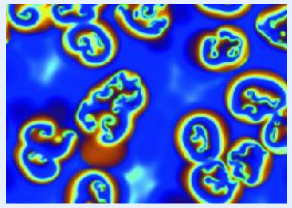


Reaction Systems

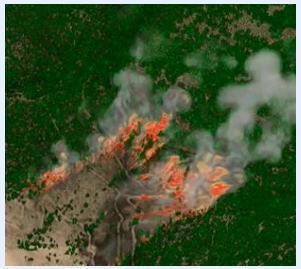
PDE-Constrained Optimization
(Space-Time)



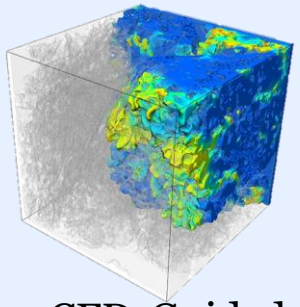
Structural Design



Diffusive Systems



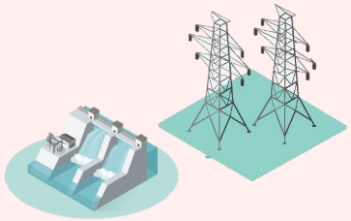
Wildfire Management



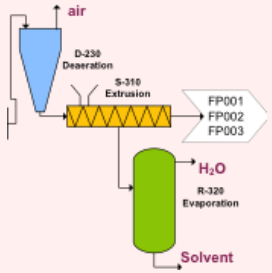
CFD-Guided Design

Stochastic Optimization
(Uncertainty)

Pharmaceutical Production



Optimal Power Flow



Process Design

Investment Planning

InfiniteOpt

Unifying Abstraction

- Captures **wide envelope** of problems
- Automates **transformations**
- Inspires **new modeling** approaches

Compact and Performant Modeling

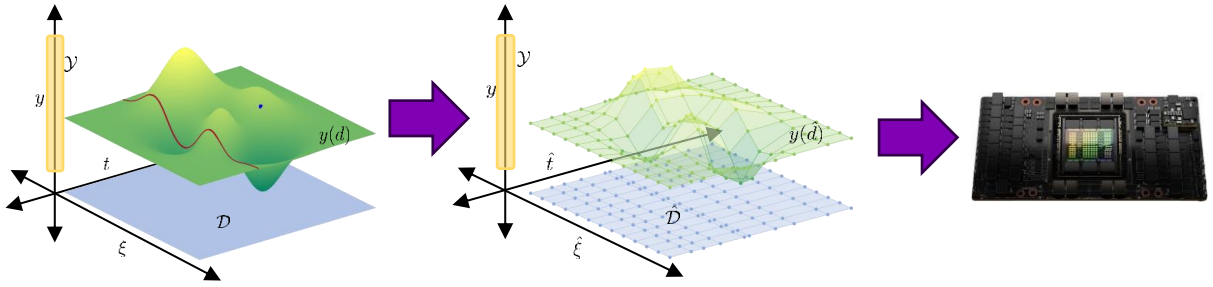
$$\frac{\partial y_b(t,\xi)}{\partial t} = 2y_b(t,\xi)^2 + y_a(t) - z_1$$

$$\mathbb{E}_\xi\left[y_c(t,\xi)\right] \geq \alpha$$

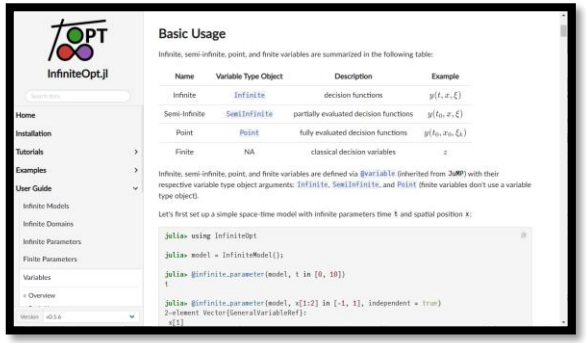
$$y_a(0) + z_2 = \beta$$

```
@constraint(m, ∂(yb, t) == 2yb^2 + ya - z[1])
@constraint(m, 𝔼(yc, ξ) ≥ α)
@constraint(m, ya(0) + z[2] == β)
```

Accelerated Solutions



Extensive Documentation



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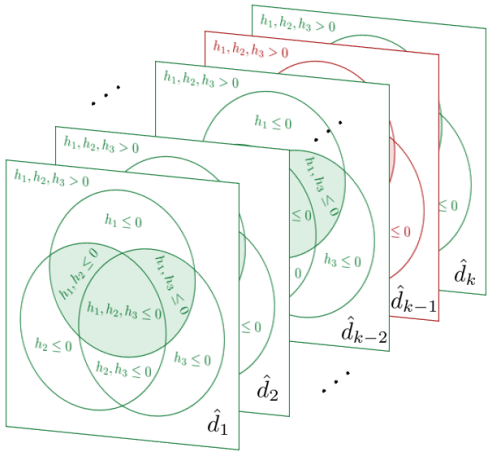
WHAT ABOUT OTHER TOOLS?

Tool	ODEs	PDEs	Stochastic	Free	Extensible	ML Models	GPU	Measures
InfiniteOpt	✓	✓	✓	✓	✓	✓	✓	✓
PyomoDAE	✓	✓	✗	✓	✓	~	✗	~
CasADi	✓	✗	✗	✓	✗	✗	✗	✗
GEKKO	✓	~	✗	✓	✗	✓	✗	✗
et	✓	✗	✗	✓	✓	✗	✓	~
gPROMS	✓	✗	✗	✗	✗	✗	✗	~
	✓	✓	✗	✓	✓	~	~	~

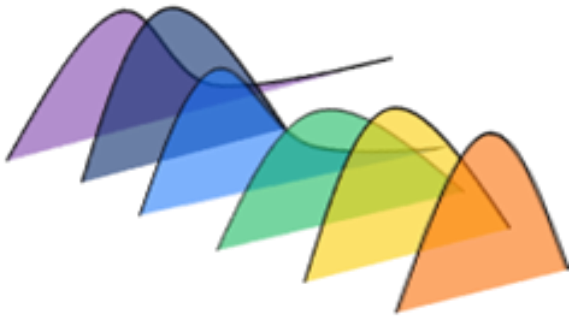
INSPIRING NEW MODELING OBJECTS

Event Constraints



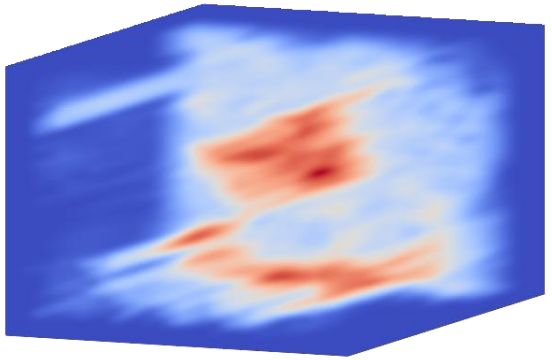
$$\mathbb{P}_d(g(y(d), z, d) \leq 0) \geq \alpha$$

Risk-Inspired Measures



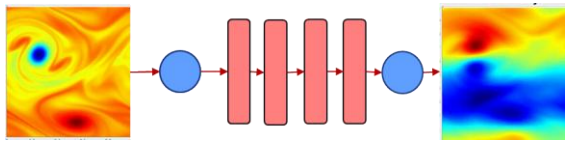
$$R(f(y(d), d))$$

Random Field Optimization



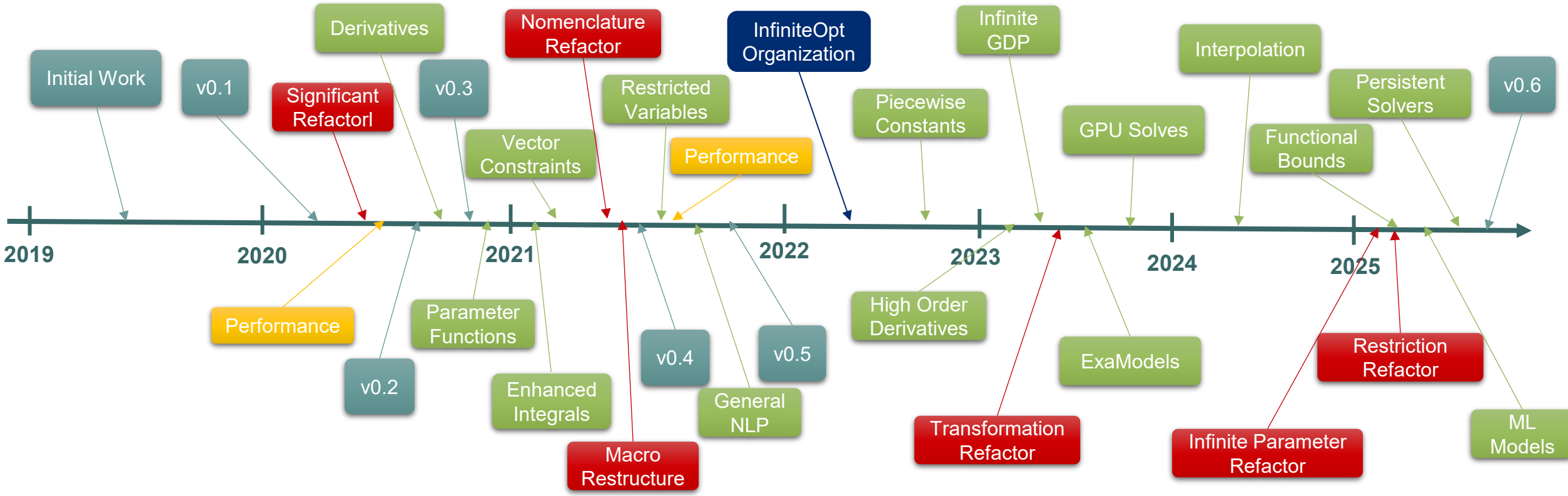
$$y(t, x, \xi(t, x))$$

Infinite-Dimensional ML Surrogates



$$NO(u(d)) = x(d)$$

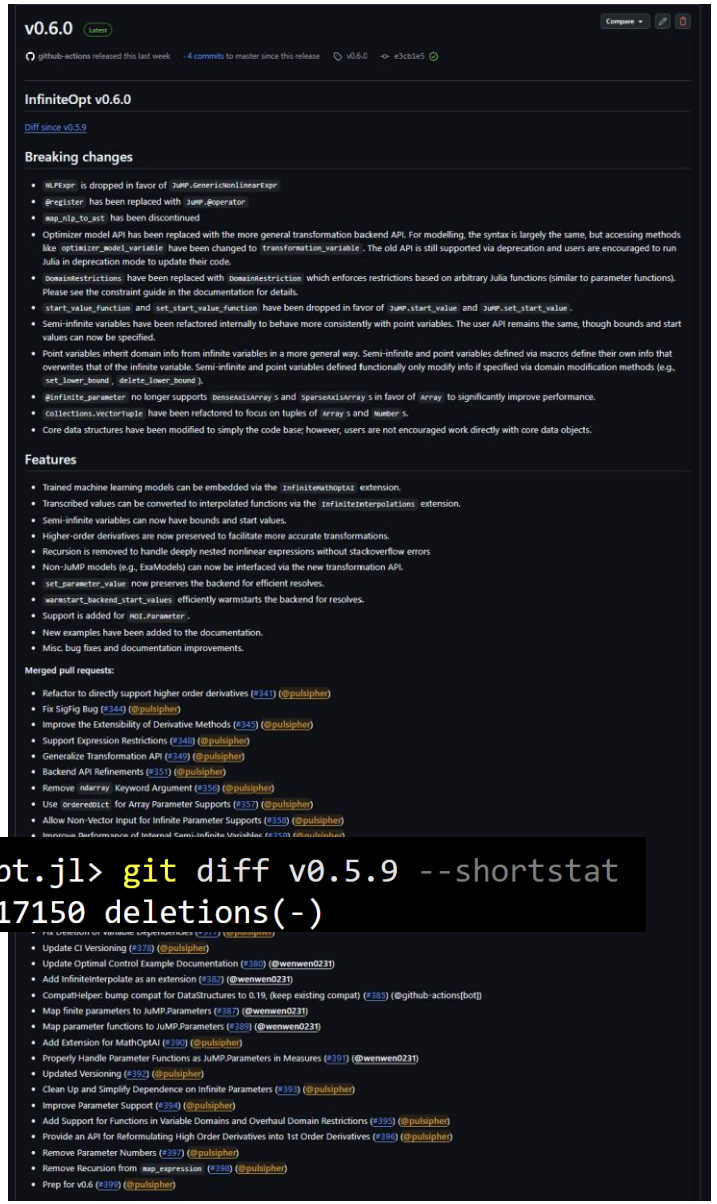
DEVELOPMENT HISTORY



WHAT'S NEW WITH VERSION 0.6?

- Extensive features/changes over past 3 years
  - User interface is largely unchanged
  - New nonlinear expressions
  - New **transformation** API
  - Refactor reduced variables
  - Functional bounds
  - **GPU accelerated solution**
  - **ML model** embedding
  - Infinite GDPs
  - Much much more

```
PS C:\Users\Pulsipher\Documents\InfiniteOpt.jl> git diff v0.5.9 --shortstat
 137 files changed, 15594 insertions(+), 17150 deletions(-)
```



v0.6.0 Latest

Compare

github-actions released this last week · 4 commits to master since this release · v0.6.0 · e3cb1e5

InfiniteOpt v0.6.0

Diff since v0.5.9

Breaking changes

- `NLPExpr` is dropped in favor of `JuMP.GenericNonlinearExpr`
- `@register` has been replaced with `JuMP.@operator`
- `map_nlp_to_ast` has been discontinued
- Optimizer model API has been replaced with the more general transformation backend API. For modelling, the syntax is largely the same, but accessing methods like `optimizer_model_variable` have been changed to `transformation_variable`. The old API is still supported via deprecation and users are encouraged to run Julia in deprecation mode to update their code.
- `DomainRestrictions` have been replaced with `DomainRestriction` which enforces restrictions based on arbitrary Julia functions (similar to parameter functions). Please see the constraint guide in the documentation for details.
- `start_value_function` and `set_start_value_function` have been dropped in favor of `JuMP.start_value` and `JuMP.set_start_value`.
- Semi-infinite variables have been refactored internally to behave more consistently with point variables. The user API remains the same, though bounds and start values can now be specified.
- Point variables inherit domain info from infinite variables in a more general way. Semi-infinite and point variables defined via macros define their own info that overwrites that of the infinite variable. Semi-infinite and point variables defined functionally only modify info if specified via domain modification methods (e.g., `set_lower_bound`, `delete_lower_bound`).
- `@infinite_parameter` no longer supports `DenseAxisArray`s and `SparseAxisArray`s in favor of `Array` to significantly improve performance.
- `Collections.VectorTuple` have been refactored to focus on tuples of `Array`s and `Number`s.
- Core data structures have been modified to simply the code base; however, users are not encouraged work directly with core data objects.

Features

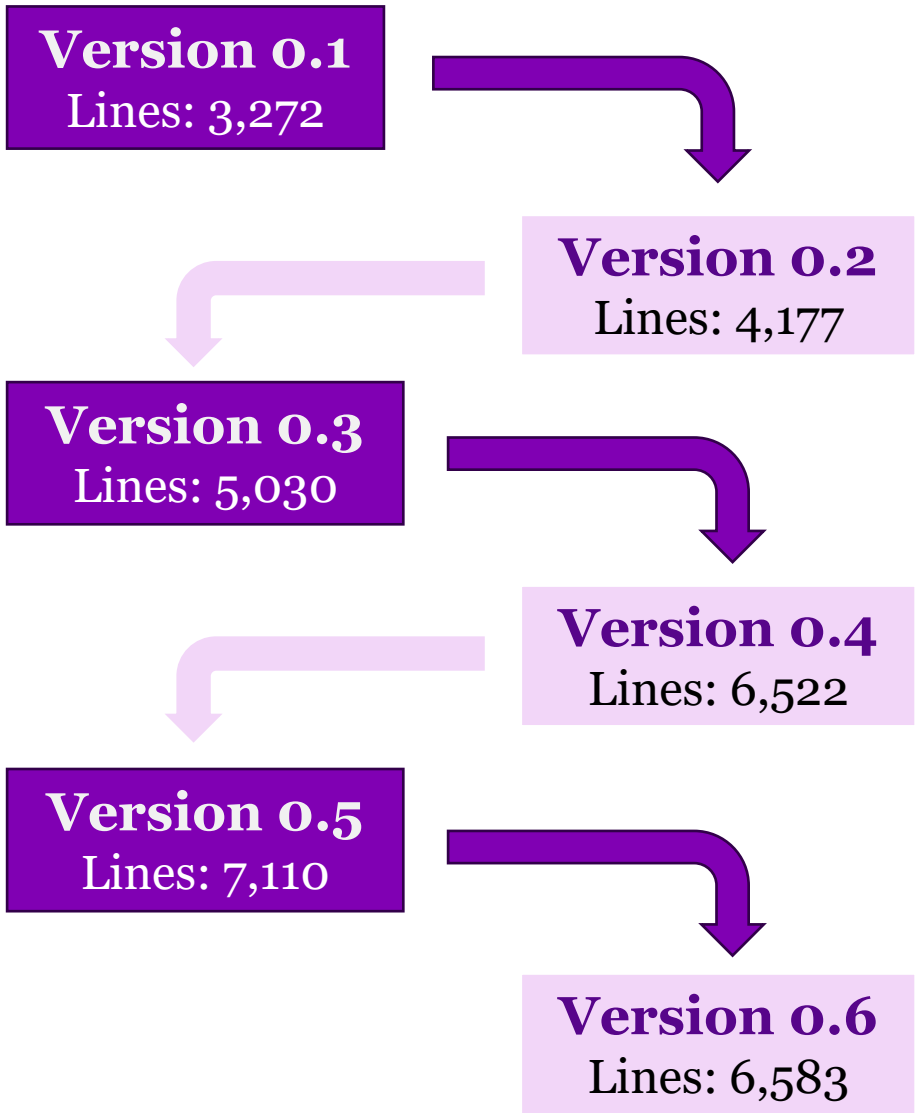
- Trained machine learning models can be embedded via the `InfiniteMathOptAI` extension.
- Transcribed values can be converted to interpolated functions via the `InfiniteInterpolations` extension.
- Semi-infinite variables can now have bounds and start values.
- Higher-order derivatives are now preserved to facilitate more accurate transformations.
- Recursion is removed to handle deeply nested nonlinear expressions without stackoverflow errors
- Non-JuMP models (e.g., ExaModels) can now be interfaced via the new transformation API.
- `set_parameter_value` now preserves the backend for efficient resolves.
- `warmstart_backend_start_values` efficiently warmstarts the backend for resolves.
- Support is added for `MOI.Parameter`.
- New examples have been added to the documentation.
- Misc. bug fixes and documentation improvements.

Merged pull requests:

- Refactor to directly support higher order derivatives (#341) (@pulsipher)
- Fix SigFig Bug (#344) (@pulsipher)
- Improve the Extensibility of Derivative Methods (#345) (@pulsipher)
- Support Expression Restrictions (#348) (@pulsipher)
- Generalize Transformation API (#349) (@pulsipher)
- Backend API Refinements (#351) (@pulsipher)
- Remove `ndarray` Keyword Argument (#356) (@pulsipher)
- Use `OrderedDict` for Array Parameter Supports (#357) (@pulsipher)
- Allow Non-Vector Input for Infinite Parameter Supports (#358) (@pulsipher)
- Update CI Versioning (#378) (@pulsipher)
- Update Optimal Control Example Documentation (#380) (@wenwen0231)
- Add InfiniteInterpolate as an extension (#382) (@wenwen0231)
- CompatHelper: bump compat for DataStructures to 0.19, (keep existing compat) (#385) (@github-actions[bot])
- Map finite parameters to JuMP.Parameters (#387) (@wenwen0231)
- Map parameter functions to JuMP.Parameters (#389) (@wenwen0231)
- Add Extension for MathOptAI (#390) (@pulsipher)
- Properly Handle Parameter Functions as JuMP.Parameters in Measures (#391) (@wenwen0231)
- Updated Versioning (#392) (@pulsipher)
- Clean Up and Simplify Dependence on Infinite Parameters (#393) (@pulsipher)
- Improve Parameter Support (#394) (@pulsipher)
- Add Support for Functions in Variable Domains and Overhaul Domain Restrictions (#395) (@pulsipher)
- Provide an API for Reformulating High Order Derivatives into 1st Order Derivatives (#396) (@pulsipher)
- Remove Parameter Numbers (#397) (@pulsipher)
- Remove Recursion from `map_expression` (#398) (@pulsipher)
- Prep for v0.6 (#399) (@pulsipher)

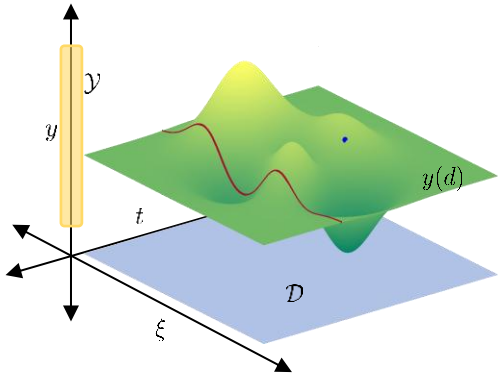
SIMPLIFIED CODE BASE

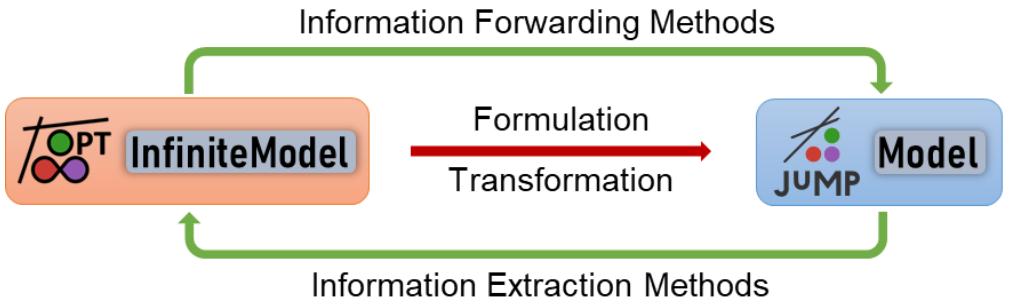
- Features and performance refactors steadily increased tracked source code lines
- **Reduced code** and increased performance
- Removed unnecessary complexity

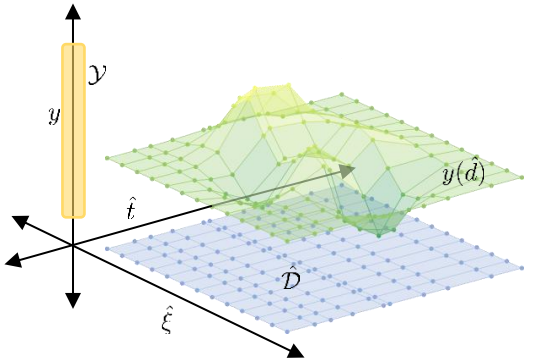


OPTIMIZER MODELS → TRANSFORMATION BACKENDS

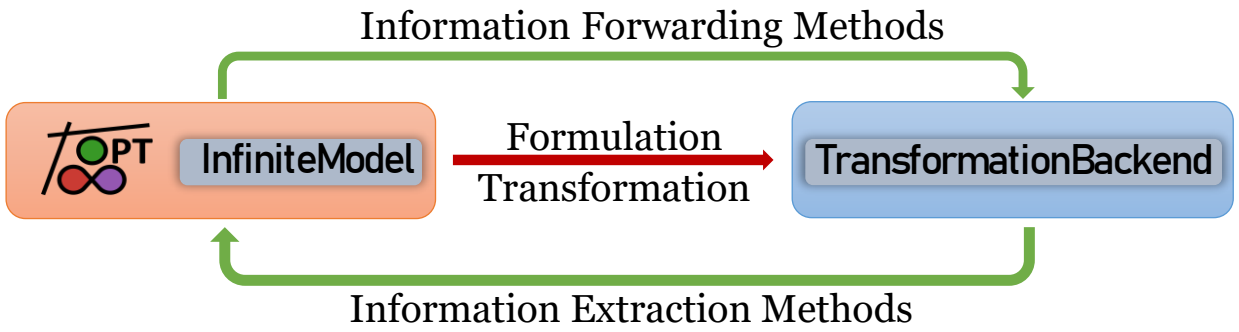
- *Before v0.6:* Optimizer model API







- *v0.6:* Transformation backend API

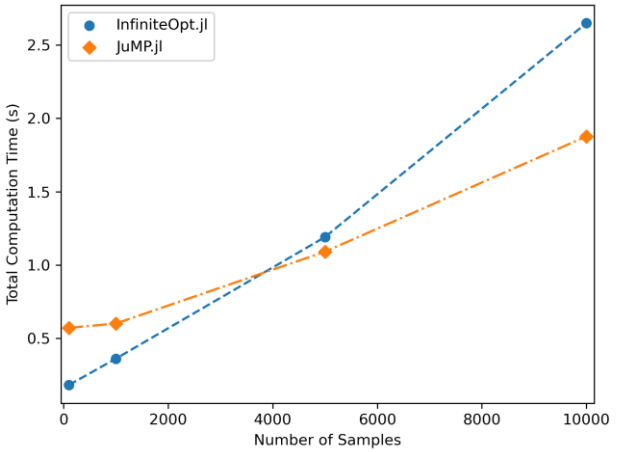


JuMP

ExaModels

IMPROVED TRANSCRIPTION

- TranscriptionOpt provides large library of discretization methods
  - E.g., finite difference, orthogonal collocation, quadrature, trapezoid, more
  - v0.6 expands library to better support higher order derivatives
- All outputs now are given as N-dimensional arrays
  - Where N is the # of infinite parameters



InfiniteOpt.jl
↓
Automatic Transcription

JuMP.jl
↓
Manual Transcription

INFINITEINTERPOLATIONS.JL

- Use interpolation to return continuous function solutions

- Extension of Interpolations.jl

- Works on variables, constraints, and expressions

```julia
using InfiniteOpt, Interpolations

# DEFINE AND SOLVE INFINITEMODEL HERE

discrete_y = value(y)
continuous_y = value(y, Constant()) # piecewise constant
continuous_y = value(y, Linear()) # linear spline
continuous_y = value(y, Cubic()) # cubic spline
```

FUNCTIONAL BOUNDS AND DOMAIN RESTRICTIONS

- Infinite variables support **function** bounds
- Semi-infinite variables now support bounds/starts
- Domain restrictions now take **arbitrary function**
  - Previously limited to subintervals
  - This is quite useful for PDEs

```
1   using InfiniteOpt
2   model = InfiniteModel()
3   @infinite_parameter(model, t ∈ [0, 10])
4   @infinite_parameter(model, x ∈ [-1, 1])
5
6   upper(t, x) = sin(t) * x
7   @variable(model, 0 ≤ y ≤ upper, Infinite(t, x))
8   set_upper_bound(y(0, x), 42)
9
10  restrict(t) = !iszero(t)
11  restriction = DomainRestriction(restrict, t)
12  @constraint(model, 3y^2 + 2y ≥ 2, restriction)
```

IMPROVED PARAMETER SUPPORT

- Previously parameter updates required rebuilding the backend
- New **persistent API** added to transformation backends
- Can update finite parameter and parameter functions (new)

```
using InfiniteOpt, Ipopt
model = InfiniteModel(
    Ipopt.Optimizer,
    update_parameter_functions = true
)
@infinite_parameter(model, t ∈ [0, 10])

@finite_parameter(model, p == 42)
@parameter_function(model, setpoint == t -> t > 5 ? 20 : 10)

# DEFINE THE MODEL

optimize!(model)

set_parameter_value(p, 10)
set_parameter_value(setpoint, t -> t > 3 ? 20 : 10)
```

WARMSTARTING

- Update start values via set_start_values
  - Uses last solution
  - **Requires Interpolations.jl** be imported
  - Backend will be rebuilt
- Update start values via warmstart_backend_start_values
  - Supports **persistent backend**
  - Updates all possible variables
  - The start values in the InfiniteModel are not updated

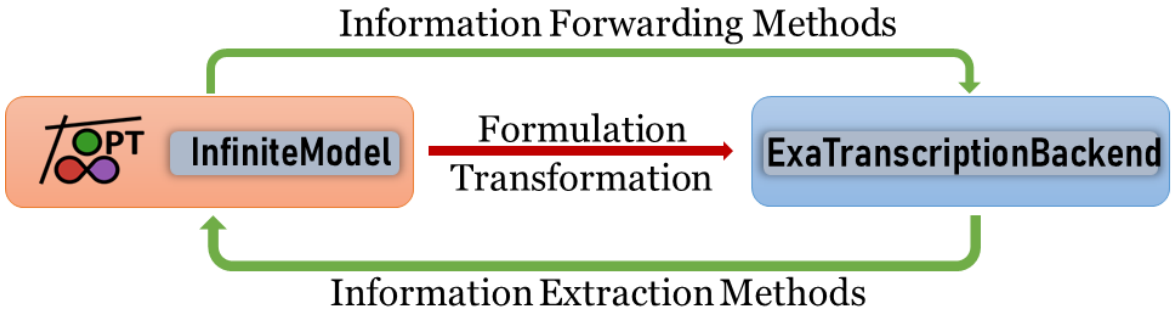
```
1   using InfiniteOpt, Interpolations, Ipopt
2   model = InfiniteModel(Ipopt.Optimizer)
3
4   # DEFINE THE MODEL
5
6   optimize!(model) # initial solve
7
8   set_start_values(model)
9
10  optimize!(model) # backend is rebuilt
11
12  warmstart_backend_start_values(model)
13
14  optimize!(model) # backend is not rebuilt
```

INFINITEEXAMODELS.JL: ACCELERATING SOLUTION

- Bridges the gap between InfiniteOpt & ExaModels
- **Automates transcription** through intuitive interface
- Leverages repeated structure to reduce **model creation time**
- Supports CPU (via Ipopt) and **GPU** (via MadNLP)

v0.1 is now released!

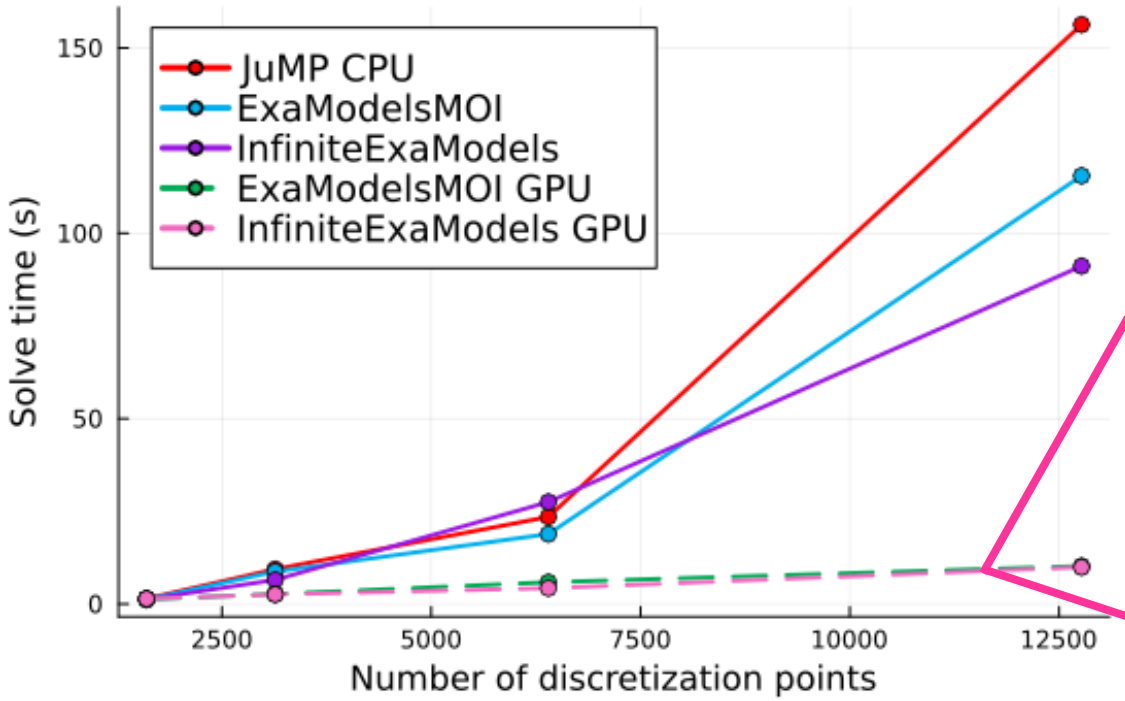
```
using InfiniteOpt, InfiniteExaModels, MadNLPGPU, CUDA
transform_backend = ExaTranscriptionBackend(MadNLPSolver, backend = CUDABackend())
model = InfiniteModel(transform_backend)
```

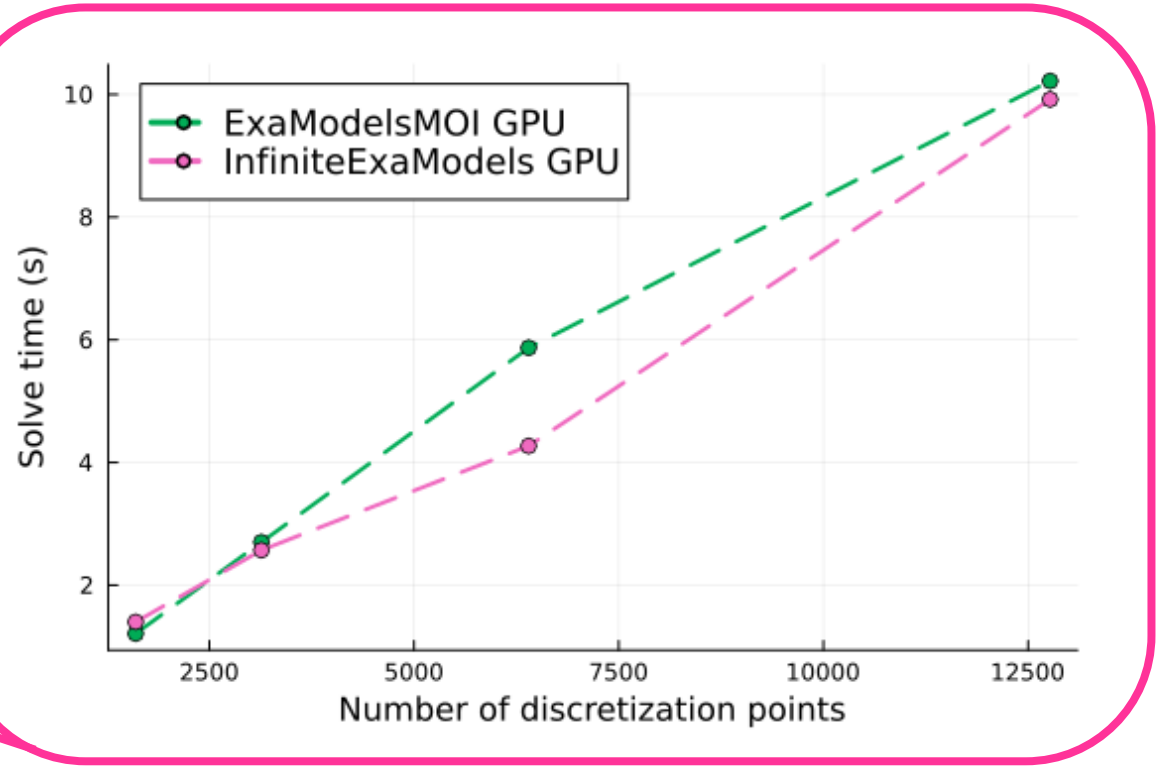


INFINITEEXAMODELS.JL: OPTIMAL CONTROL

Paper

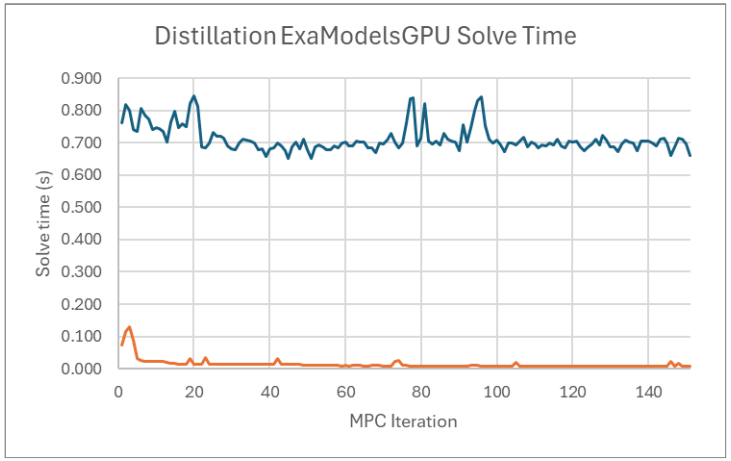
- GPU performs & scales better than CPU workflows
  - Significant time spent for **solver initialization**





RAPID NONLINEAR MODEL PREDICTIVE CONTROL

- New persistent backend + InfiniteExaModels.jl + GPU → **fastest known NMPC**



0.71 s per iteration

0.01 s per iteration

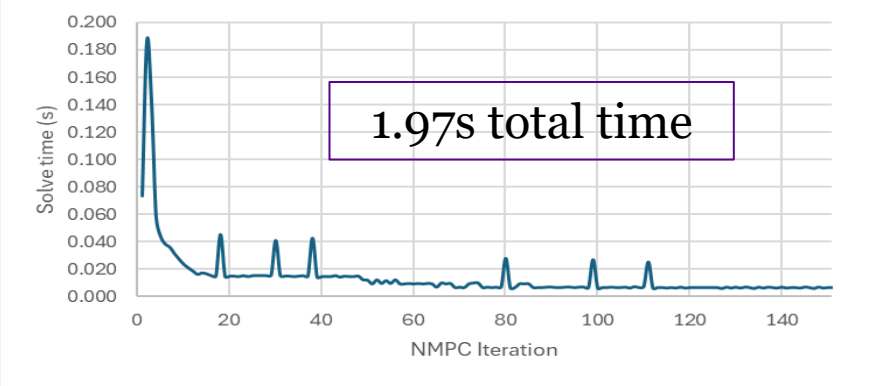
```julia
using InfiniteOpt, Ipopt
model = InfiniteModel(Ipopt.Optimizer)
# DEFINE THE MODEL

for i in 1:N
    optimize!(model)
    warmstart_backend_start_values(model)
    set_parameter_value(x0, value(x(0)))
    set_parameter_value(setpoint, set[i])
end
```

	JuMP		ExaModelsCPU		ExaModelsGPU	
Case Study	**Base**	**WS + PU**	**Base**	**WS + PU**	**Base**	**WS + PU**
Distillation	137.53	39.09	61.45	17.08	30.94	1.62
PDE Heated Plate	143.95	135.19	136.35	80.31	21.53	1.42

OPTIMALCONTROL.JL VS. INFINITEOPT.JL FOR NMPC

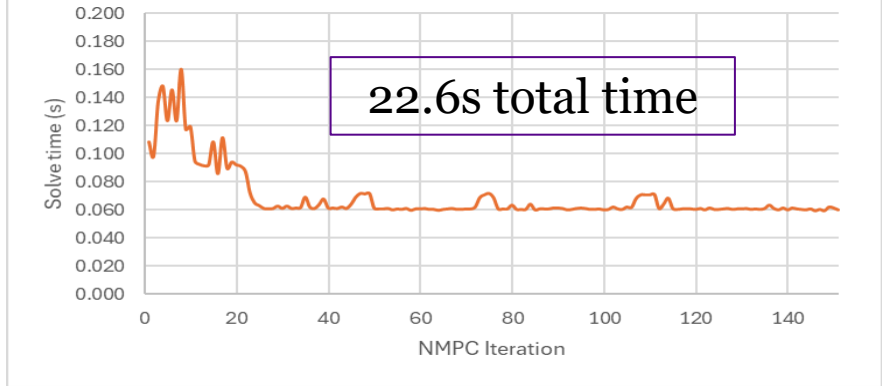
InfiniteOpt.jl

- Interfaces with ExaModels → GPU NMPC
- Supports ODEs and **PDEs**
- Supports **orthogonal collocation** and finite difference on GPU
- Support **set notation** (benchmark 22 lines)
- Supports **persistent solves**



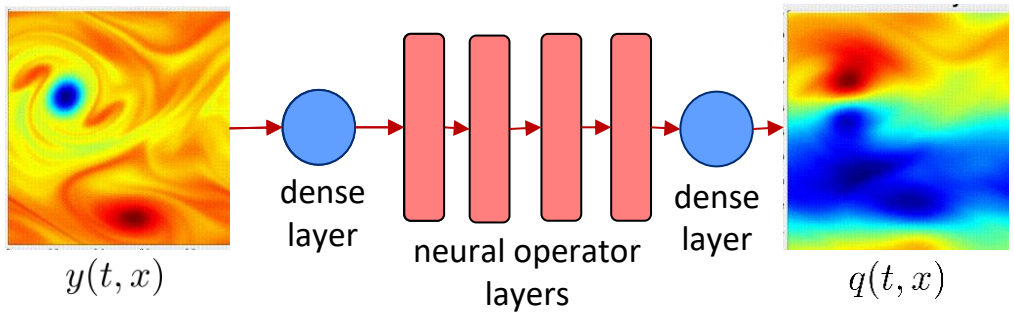
OptimalControl.jl

- Interfaces with ExaModels → GPU NMPC
- Supports ODEs
- Supports **only finite difference** on GPU
- Doesn't support set notation (benchmark **63 lines**)
- **Rebuilds solver** instance



INFINITEMATHOPTAI.JL: EMBEDDING ML MODELS

- Acts as a bridge between InfiniteOpt & MathOptAI.jl
- **Embed ML models** directly in InfiniteOpt problems
- Enables use of **neural ODEs**
- Opens possibility for infinite ML models
  - Gaussian processes
  - Neural operators




```julia
using InfiniteOpt, Flux, MathOptAI
NN = predictor(
    Flux.Chain(
        Flux.Dense(2, 16, Flux.relu),
        Flux.Dense(16, 16, Flux.relu),
        Flux.Dense(16, 2)
    )
)
model = InfiniteModel()
@infinite_parameter(model, t ∈ [0, 10])
@variable(model, x[1:2], Infinite(t))
y, formulation = add_predictor(model, NN, x)
@constraint(model, [i in 1:2], ∂(x[i], t) == y[i])
```

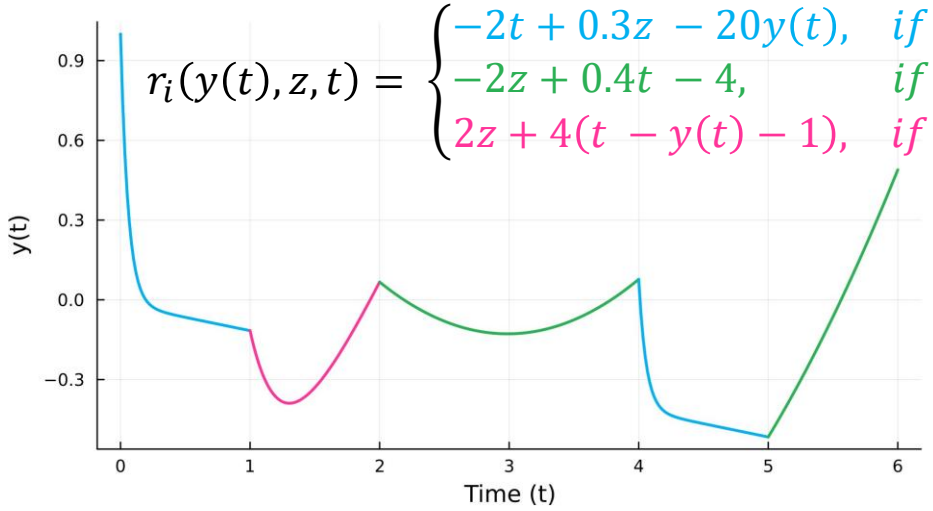
INFINITEDISJUNCTIVEPROGRAMMING.JL: MODELING LOGIC

- Enables infinite-dimensional GDP
- Model ODE/constraint switching

Paper

InfiniteOpt + JuMP

$$r_i(y(t), z, t) = \begin{cases} -2t + 0.3z - 20y(t), & if\ i = 1 \\ -2z + 0.4t - 4, & if\ i = 2 \\ 2z + 4(t - y(t) - 1), & if\ i = 3 \end{cases}$$




```julia
using DisjunctiveProgramming, InfiniteOpt, HiGH
model = InfiniteGDPModel(HiGHS.Optimizer)
I = 1:4; J = 1:2
@infinite_parameter(model, t ∈ [0, 1], num_supports = 100)
@variable(model, 0 ≤ y[I] ≤ 10, Infinite(t))

# Add the disjunctions and their indicator variables
@variable(model W[I, J], InfiniteLogical(t))
@constraint(model, [i ∈ I, j ∈ J], 0 ≤ y[i], Disjunct(W[i, 1]))
@constraint(model, [i ∈ I, j ∈ J], y[i] ≤ 0, Disjunct(W[i, 2]))
@disjunction(model, [i ∈ I], W[i, :])

# Add the logical propositions
@constraint(model, W[1, 1] ∨ W[2, 1] ∧ W[3, 1] := true)
optimize!(model, gdp_method = Hull())
```

MTKINFINITEOPTEXT.JL: INTEGRATING MTK MODELS

- Ports ModelingToolkit models to InfiniteOpt
- Enables structural simplifications
- More work is needed to increase performance and better use InfiniteOpt's extension API

```julia
using ModelingToolkit, InfiniteOpt, Ipopt

# Double integrator minimum time
t = M.t_nounits
D = M.D_nounits
@variables x(..) v(..)
@variables u(..) [bounds = (-1.0, 1.0), input = true]
@parameters tf
constr = [v(tf) ~ 0.0, x(tf) ~ 0]
cost = [tf] # Maximize the final distance.
@named block = ODESystem(
    [D(x(t)) ~ v(t), D(v(t)) ~ u(t)], t; costs = cost, constraints = constr)
block, input_idxs = structural_simplify(block, ([u(t)], []))

u0map = [x(t) => 1.0, v(t) => 0.0]
tspan = (0.0, tf)
parammap = [u(t) => 0.0, tf=>1.0]
jprob = JuMPDynamicOptProblem(block, u0map, tspan, parammap; steps = 51)
jsol = solve(jprob, Ipopt.Optimizer, :Verner8)
```

DEVELOPMENT ROADMAP (A PARTIAL SNAPSHOT)

- Add more features that JuMP supports
  - Multi-objective, generic precision, complex values, etc.
- Enhance PDE support (e.g., support finite elements)
- Expand envelope of persistent backend API
- Develop GPU-accelerated parameter estimation workflows
- Infinite ML models
  - Add support for larger collection of infinite-dimensional ML models
  - Use simultaneous method to train neural ODEs
- Infinite GDP: Finish release and develop tailored solver

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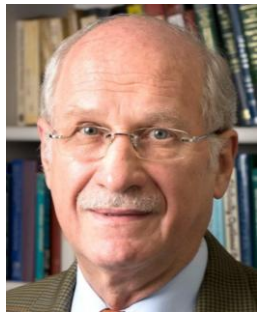

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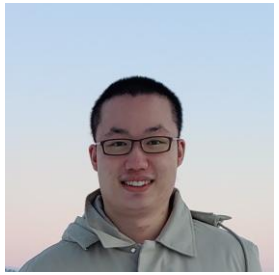

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TRY IT OUT!

InfiniteExaModels.jl

InfiniteOpt

DisjunctiveProgramming.jl