VERICOMP: Comparing and Recommending Verified IVP Solvers

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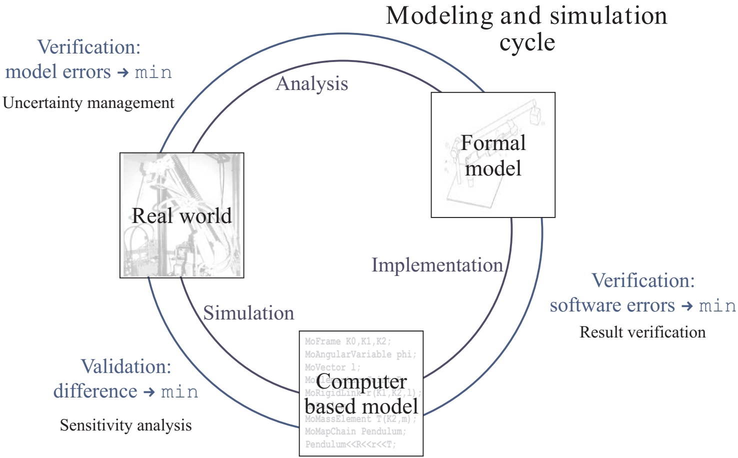
Modeling/Simulation vs Verification/Validation



Result Verification

Features:

- Prove the correctness of the computed result
- Take into account rounding or conversion errors
- Account for the epistemic uncertainty (e.g. in measurements)

Approaches:

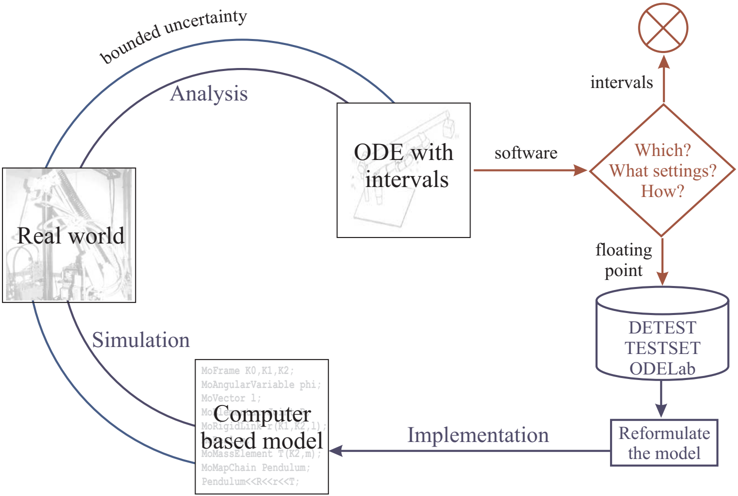
- interval and affine arithmetics,
- Taylor models, ...

Beginnings:

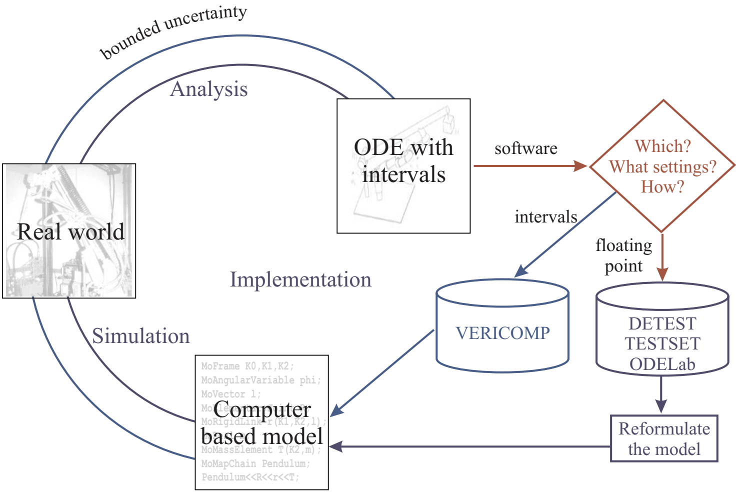
- Dissertation by R. E. Moore, 1962

Result verification might help where other V&V techniques fail!

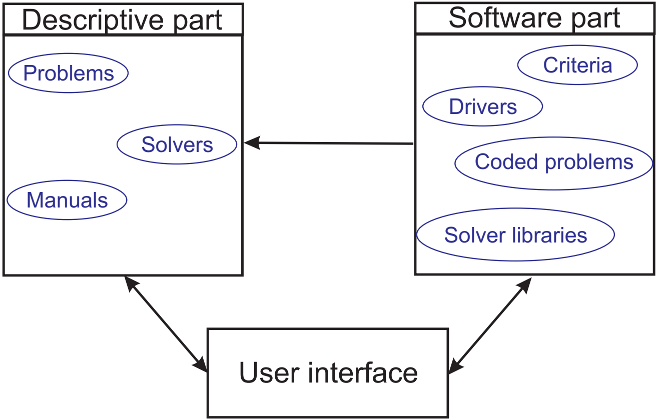
Comparison of IVP Solvers



Comparison of IVP Solvers



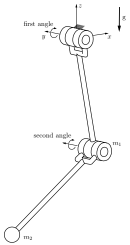
Comparison of Floating-Point-Based Solvers

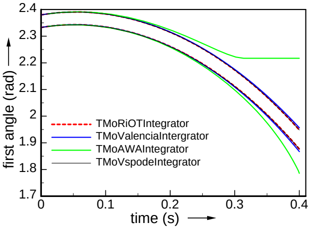


DETEST/StiffDETEST, TESTSET, ODELab

Peculiarities of Comparing Verified Solvers

Example: A double pendulum with an uncertain initial angle





- different performance for problems with or without uncertainty
- the answer is an interval with a non-zero diameter
- possible break-down
- the answer is always reliable

How Can VERICOMP Be of Use?

Scenario 1: Find the optimal solver for a problem

→ (or get a solver recommended)

Scenario 2: Compare the performance of your newly developed verified IVP solver with the existing ones (VNODE-LP, RiOT, ValEncIA-IVP)

Scenario 3: Collaborative analytics like ARCH-COMP

We show an application example for Scenario 1!

A Possibility for VERICOMP's Application

ARCH Workshop — Applied verification for continuous and hybrid systems

$\rightarrow$ Within the National Science Foundation-funded Cyber-Physical Systems Virtual Organization (CPS-VO)

One aim: Establishing a curated set of benchmarks submitted by academia and industry in the area

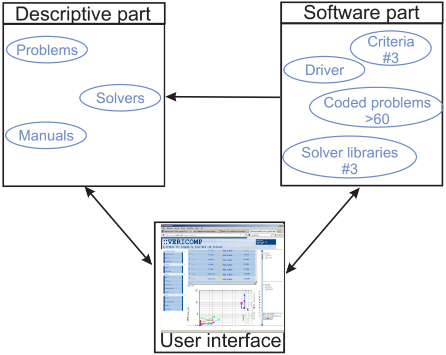
Topics:
- Proposals for new benchmark problems; tool presentations
- Tool executions/evaluations based on ARCH benchmarks
- Experience reports including open issues for industry

Part of activities: A competition `cps-vo.org/group/ARCH/FriendlyCompetition`

Workflow: Join a group $\rightarrow$ determine the set of problems (ARCH pdf repository) $\rightarrow$ submit results (via e-mail) $\rightarrow$ prepare a report $\rightsquigarrow$ Manual!

VERICOMP would automate this workflow!

Framework VERICOMP: Stucture and History



University of Duisburg-Essen

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Online since 2010

↓

Mainly volunteered work

`vericomp.inf.uni-due.de`

↓

Hardware damage 2015

↓

Since 2017: reconstruction

`vericomp.fiw.hs-wismar.de`

↓

New design online (for problems) 🙂

Used by developers of verified IVPS (e.g. DynIBEX 2016)

Dzetkulic, T.(2015). Rigorous integration of non-linear ordinary differential equations in Chebyshev basis. Numer. Alg. 69.1
dit Sandretto, J.;A. Chapoutot (2016). Validated Explicit and Implicit Runge-Kutta Methods. In: Reliable Computing 22.

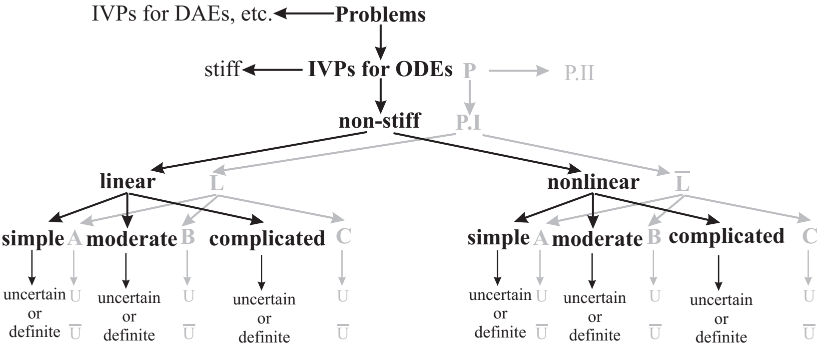
Theoretical Basis: Problems

(Nonstiff) Initial value problems of the form:

$$\dot{x}(t) = f\big(x(t)\big), \quad x(t_0) \in \left[x^0\right] \quad ,$$

- $t_0 = 0$, $t \in [0; t_f] \subset \mathbb{R}$ for some $t_f > 0$
- $\left[x^0\right] = \left[\underline{x}^0 \, ; \, \overline{x}^0\right]$
- f can depend on parameters p with $[p] = \left[\underline{p} \, ; \, \overline{p}\right]$
- the problem is discretized
- the solution is $[x_k]$ with $x(t_k; 0, [x_0]) \subseteq [x_k]$

Problems: Classification



Theoretical Basis: Criteria

C1 Number of arithmetic operations at a time step

C2 Number of function/ Jacobian, etc./ inverse matrix evaluations

C3 Overhead

C4 Wall clock time

C5 User CPU time wrt. overestimation

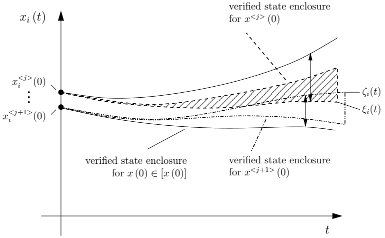
C6 Time to break-down t_{bd} for each solver

C7 Total number of steps and number of accepted steps.

Each criteria can be weighted according to the application.

Characterization of Overestimation for C5

1. Analytical solution $x(t)$: $\max_{i=1}^{n}\{\mathsf{d}([x_k]_i) - \mathsf{d}(x_i(t_k))\}$
2. No uncertainty: $\max_{i=1}^{n} \mathsf{d}([x_k]_i)$
3. *Uncertainty in parameters:* $\max_{i=1}^{n}\{|\overline{x_i} - \xi_i| + |\underline{x_i} - \zeta_i|\}$



Statistics

→ Tables

→ Work-precision diagrams

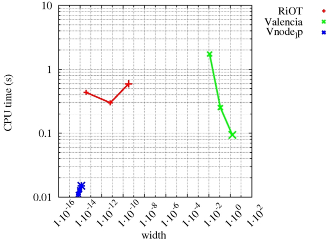
→ Solution plots

Possible:

→ Spider diagrams

→ ...

A WPD for ID 19 (formerly)



::VERICOMP

A System for Comparing Verified IVP Solvers

UNIVERSITÄT DUISBURG ESSEN

ID: 19
Equations
x0'= 2.0*x0-2.0*x0*x1 x1'= -x1+x0*x1
Initial Values
1 3
Parameters
[--/--]
Class
PINLBNU
Exact Solution
--/--
Description
B1 from DETEST

show/hide statistics

Statistics

→ Tables

→ Work-precision diagrams

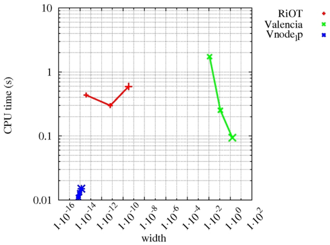
→ Solution plots

Possible:

→ Spider diagrams

→ ...

A WPD for ID 19 (formerly)



RiOT

settings	c1	c2	c3	c4	c5_time	c5_width	c6_time	c6_width	c7.1	c7.2
Order=10 Bounder =LDB Sparsity =1e-15 Step cntrl =AUTO h start =2e-2 h min =2e-3 Local error tol =1e-11	-/-	-/-	-/-	0m0.316s	0m0.300s	6.5050187458837E-12	- +1.0000000000000000E+01	0.057420587925039	-/-	-/-

results from new problem
19/RiOT__Order_=0__Bounder_=__Sparsity_=__Step_cntrl_=__h_start_=__h_min_=__Local_error_tol_=__.txt
19/RiOT__Order_=10__Bounder_=LDB__Sparsity_=1e-15__Step_cntrl_=AUTO__h_start_=2e-2__h_min_=2e-3__Local_error_tol_=1e-11__.txt

Valencia

settings	c1	c2	c3	c4	c5_time	c5_width	c6_time	c6_width	c7.1	c7.2
Stepsize0.005	-/-	-/-	-/-	0m0.760s	0m0.754s	0.2402912925	2.3150000000e+00	1.60616223387	-/-	-/-

results from new problem
19/Valencia__Stepsize0.005.txt

Vnode_lp

settings	c1	c2	c3	c4	c5_time	c5_width	c6_time	c6_width	c7.1	c7.2
Order = 20 Tolerance = 1e-11 Hmin = 1e-6	-/-	-/-	-/-	0m0.064s	0m0.058s	2.9976021664879E-14	10.000000	1.3575318646986E-10	-/-	-/-

results from new problem
19/Vnode_lp__Order=20__Tols=1e-11__Hmin=1e-6__.txt

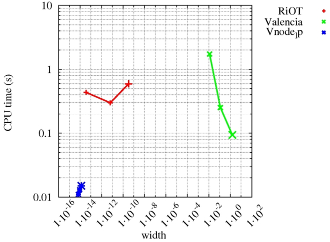
Statistics

- → Tables
- → Work-precision diagrams
- → Solution plots

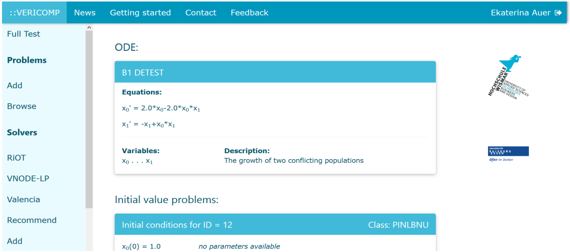
Possible:

- → Spider diagrams
- → ...

A WPD for ID 19 (formerly)



New design



Recommender: Formulation in VERICOMP

$$\max\{utility(U,K,G)\} \quad \text{with} \quad K=(P,E,S)$$

	Meaning	Meaning in VERICOMP
U	User	Problem
E	Entity set	Solvers
G	Recom. items from E	Recommended solvers
K	Context	$K=(P,S)$ (E is not dynamic)
P	User profile	Problem characteristics $\rightarrow$ classification
S	Situation	Applications (e.g. online/offline)
	Utility function	$\sum_{i=1}^{7} w_i n(C_i(g))$, $g \in G$, $\sum_{i=1}^{7} w_i = 1$

Method: Multiattribute utility collaborative filtering with C1-C7 ($C_i(g)$) and weighting w_i according to S

Illustration: Biological Wastewater Treatment

Simplified ASM1

$$\dot{S} = \frac{Q_\mathrm{W}}{V_\mathrm{A}} \left(S_\mathrm{W} - S\right) - \mu\left(S, S_\mathrm{O}\right) \frac{1}{Y} X$$

$$\dot{X} = -\frac{Q_\mathrm{W}}{V_\mathrm{A}} X + \frac{Q_\mathrm{RS,nom}}{V_\mathrm{A}} \left(X_\mathrm{Set} - X\right) + \left(\mu\left(S, S_\mathrm{O}\right) - b\right) X + \frac{Q_\mathrm{RS,nom}}{V_\mathrm{A}} \left(X_\mathrm{Set} - X\right) \Delta Q_\mathrm{RS}$$

$$\dot{S}_\mathrm{O} = \frac{Q_\mathrm{W}}{V_\mathrm{A}} \left(S_\mathrm{OW} - S_\mathrm{O}\right) - \mu\left(S, S_\mathrm{O}\right) \frac{1-Y}{Y} X + \frac{\rho_\mathrm{O2}}{V_A} \left(1 - \frac{S_\mathrm{O}}{S_\mathrm{O,sat}}\right) u_\mathrm{O2}$$

$$\dot{X}_\mathrm{Set} = \frac{Q_\mathrm{W} + Q_\mathrm{RS,nom}}{V_\mathrm{Set}} X - \frac{Q_\mathrm{EX} + Q_\mathrm{RS}}{V_\mathrm{Set}} X_\mathrm{Set} + \frac{Q_\mathrm{RS,nom}}{V_\mathrm{Set}} X \Delta Q_\mathrm{RS}$$

Growth rate of bacteria: $\mu\left(S, S_\mathrm{O}\right) = \hat{\mu}_\mathrm{H} \frac{S}{S+K_\mathrm{S}} \frac{S_\mathrm{O}}{S_\mathrm{O}+K_\mathrm{OS}}$

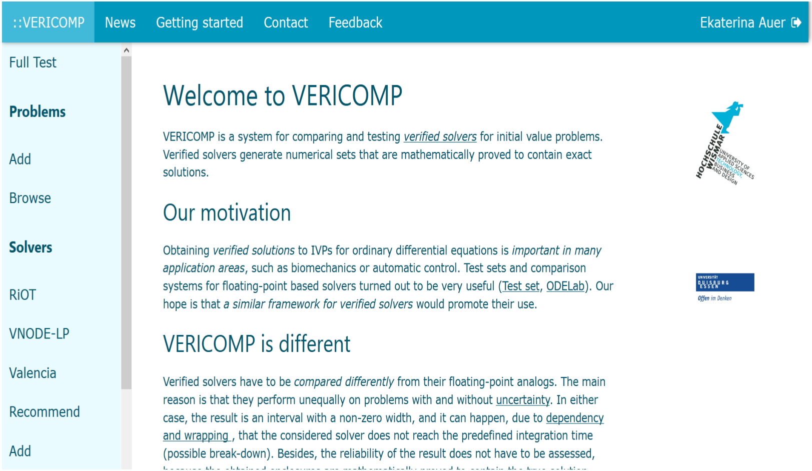
Uncertain parameters:

1. the maximum bacteria growth rate $\hat{\mu}_\mathrm{H}$
2. inflow concentration S_W of substrate
3. the initial system states

Task: Prevent dying of bacteria; ensure efficient purification with small S

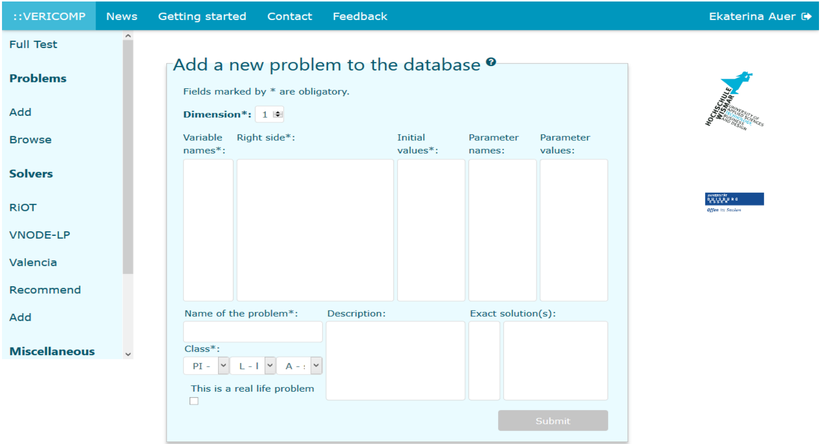
Find the Right Software in VERICOMP!

Step 0: Call VERICOMP



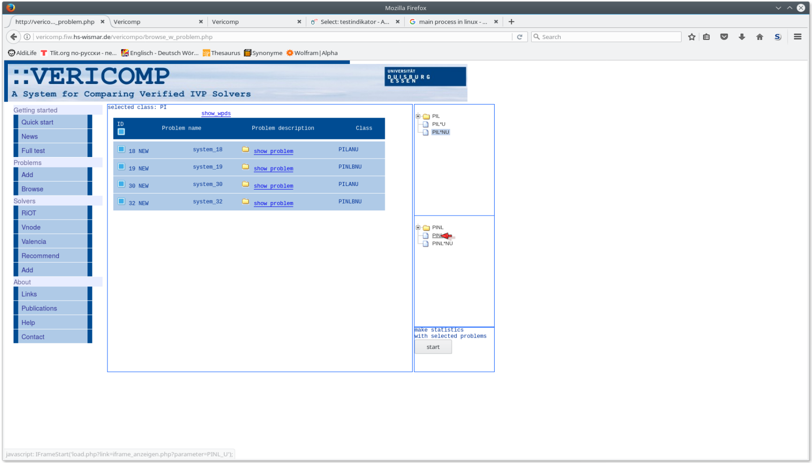
Find the Right Software in VERICOMP!

Step 1: Add to the Database



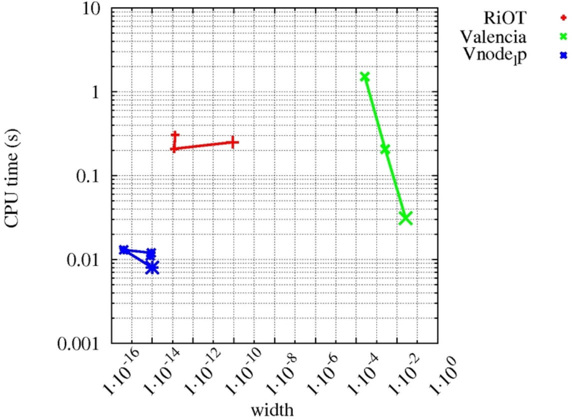
Find the Right Software in VERICOMP!

Step 2: Make Tests (Old Design)



Find the Right Software in VERICOMP!

Step 3: Compare Results



Valencia-IVP with stepsize 0.025,0.0025,0.0005

VNODE-LP with the order 10, 15, 20

RiOT with the order 5, 10, 12

Also possible: Get a solver recommended without time consuming tests!

Conclusions

Results:

- The conceptual basis for comparisons of verified IVPS developed
- A problem/solver/statistics database (re)constructed
- The recommender formalism developed

Future work:

- Full functionality with improved user interface
- Implementation of the recommender
- Possibility to add a new solver semi-automatically