An Environment for Verified Modeling and Simulation of Solid Oxide Fuel Cells

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Modeling, Simulation and Control of Solid Oxide Fuel Cells

SOFCs: devices converting chemical energy in electricity

+ high efficiency, flexibility wrt. fuel
– high operating temperature

Our goals:

- Models better suitable for control
- Verified methods for robustness
- Modeling/simulation/control in `VeriCell`

VerIPC-SOFC Project

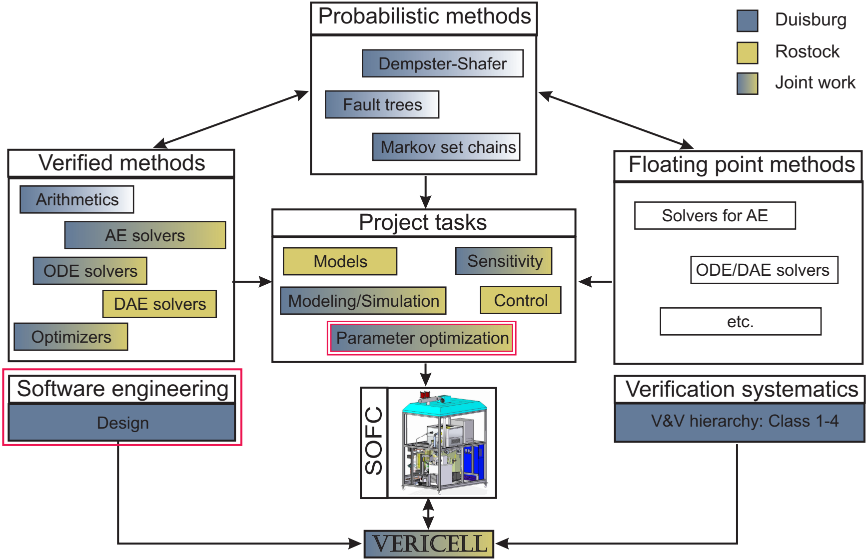
A joint project between the Universities of Rostock and Duisburg-Essen

Development of the flexible software `VeriCell`

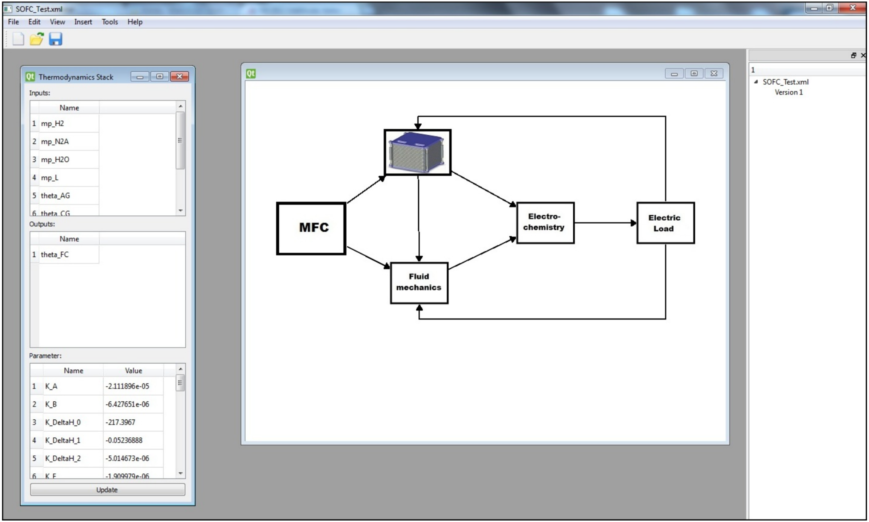
Task	**Method**
Use of different SOFC models Interfacing of existing solvers	Model abstraction, Plugins
Parameter Optimization	Global optimization
SOFC simulation and control	ODE solver, DAE solver

→ Allow for using verified and non-verified methods

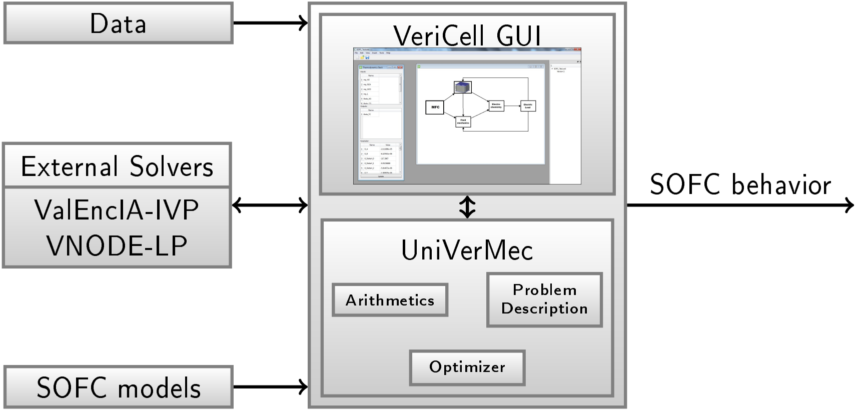
Project Overview



VeriCell GUI



Software Architecture



Ingredients of an SOFC Model Component

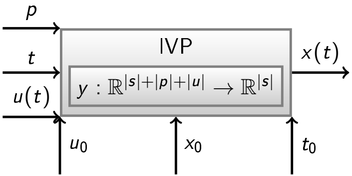
Model equation (IVP):

$$\dot{x}(p, u(t), t) = \underbrace{f\,(x(t), p, u(t))}_{y:\mathbb{R}^{|s|+|p|+|u|}\rightarrow\mathbb{R}^{|s|}}$$

depends on

t	Time
p	Parameters
$u(t)$	Dependent parameters
$s := x(t)$	Model states

Abstract IVP class



Values for

Starting time t_0

$u_0 = u(t_0), p_0 = p$

$x_0 = x(t_0)$

Acts as a basis for

- simulation
- parameter optimization

Solving the IVPs (Simulation)

Information needed by an IVP solver

IVP

End time t_{end}

Solver's specific options S_o

Possible solvers

Euler's method

ValEncIA-IVP

Needs derivatives of y

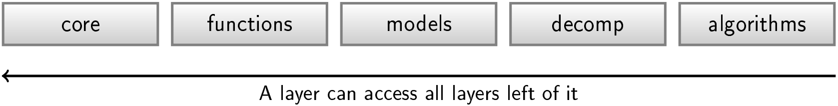
VNODE-LP

Needs Taylor coefficients of y and its Jacobian

How to represent an IVP (and y) for use with different solvers?

UniVerMeC

Unified Framework for Verified GeoMetric Computations



Uniform handling of verified techniques through a relaxed layer structure

- core: *Adapter for underlying arithmetic libraries*
- functions: *Uniform representation for functions*
- models: *IVP models*, Implicit surfaces, CSG models
- decomp: *Multisection schemes*, Spatial decomposition
- algorithms: *Global optimization*, *IVP solver interfaces*

Application in VeriCell

algorithms — Algorithms built upon the framework
→ Global optimization; VNODE-LP interface; ValEncIA-IVP interface

trees — Uniform interval tree representation

section — Multisection schemes and box management
→ Naive/Ratz multisection; Coordinate direction weights | Standard interval trees; Contracting trees

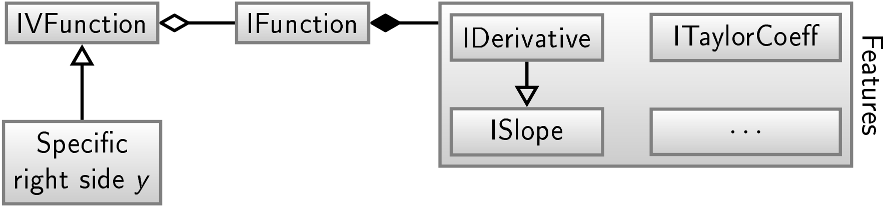
objects — Uniform geometric object representation

ivp_models — IVP model representation
→ SOFC models | Implicit objects/CSG-operations; Polyhedrons/parametric objects; Deformations/transformations

functions — Uniform function representation
→ Model right hand side; Derivatives; Taylor coefficients

core — Uniform interfaces for arithmetics
→ Real/interval/affine arithmetic; Taylor models; Matrices and vectors

Representation of the Model's Right Hand Side



Right side $y : \mathbb{R}^n \to \mathbb{R}^{|s|}$ mapped to `IVFunction`

$|s|$ member functions $f : \mathbb{R}^n \to \mathbb{R}$ offer optional *features*

The interfaces

- *hide* how y is really computed
- *hide* how derivatives are computed
- *allow* evaluation with different arithmetics

Interfacing the Solvers

Euler's Method ("Verified Approximation")

$$\mathbf{y}_k := \mathbf{y}_{k-1} + h \cdot f(\mathbf{y}_{k-1}, p)$$

→ Directly implemented in `UniVerMeC`

VNODE-LP (Verified)

1. Adapter for arithmetic compatibility to `UniVerMeC`
2. Implement VNODE's abstract `AD` interface

→ Both steps are possible thanks to VNODE's architecture

ValEnclA-IVP

ValEnclA-IVP
is coupled with libraries:

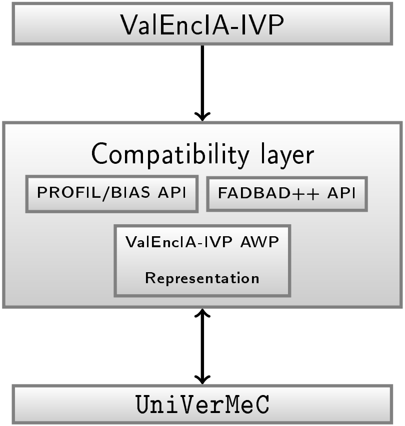
1. fadbad++
2. PROFIL/BIAS

$\rightarrow$ Compatibility layer necessary

Not thread-safe
(ValEnclA-IVP uses global variables)

In our version
no recompiling for each problem

decoupled from specific libraries

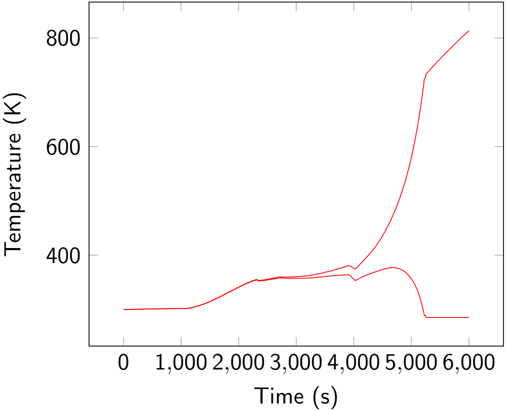


Solver Results

Problem
thermodynamics $1 \times 1 \times 1$

IC
$\theta(0) = 299.7053$
$p = (p_1, \ldots, p_{23})$
$u(t)$ from measurement file

Solver
ValEncIA (h=1)



Parameter Identification

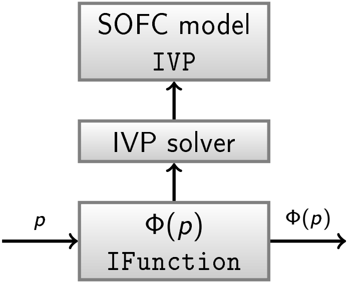
Goal

Parametrize the model for temperature in a robust and accurate way.

$$\Phi(p) = \sum_{k=1}^{T} (y(t_k, p) - y_m(t_k))^2$$

with

$p \rightarrow$ Parameters to identify
$y(t_k, p) \rightarrow$ Simulated temperature at time t
$y_m(t_k) \rightarrow$ Measured temperature at time t
$T \rightarrow$ Number of measurements (19963)
$t_{k-1} - t_k = 1s \rightarrow$ Step size 1s



→ Can be performed using different models/IVP solvers.
(Currently, we use Euler's method.)

Prolem Statement

Optimization problem

$$\min_{p \in \boldsymbol{p}_0} \Phi(p)$$

Bound constraint problem ($\boldsymbol{p}_0 \in \mathbb{IR}^6, \operatorname{wid} \boldsymbol{p}_0 = 2.0$)
Initial vector for $\boldsymbol{p}_0$ derived by floating-point methods

Difficulties

- Objective function is computationally expensive
- Calculating derivatives is really slow (even with `fadbad++`)
- Considerable overestimation

$\rightarrow$ Individual strategies for dealing with the problem (derivative free).

Consistent States

Consistent parameter vectors

A state vector $\boldsymbol{p}$ is consistent if $\forall t \in \{0, ..., T\}$:

$$[y(t, \boldsymbol{p})] \subseteq y_m(t) + [\Delta y_m]$$

with the worst-case measurement error $[\Delta y_m] = [-15, 15]$ holds.

Inconsistent parameter vectors

A state vector $\boldsymbol{p}$ is inconsistent if $\exists t \in \{0, ..., T\}$:

$$[y(t, \boldsymbol{p})] \cap (y_m(t) + [\Delta y_m]) = \emptyset$$

Branch & Bound

Basic pattern

1. $\boldsymbol{p} \leftarrow \mathcal{L}$
2. `Discard` $\boldsymbol{p}$ `if it is infeasible`
3. `Discard` $\boldsymbol{p}$ `if` $\underline{\Phi(\boldsymbol{p})} > \overline{D}$
4. `Contract` $\boldsymbol{p}$
5. `Update of` $\overline{D}$
6. `Add` $\boldsymbol{p}$ `to` $\mathcal{L}_{\text{final}}$ `if termination criteria are satisfied`
7. `Split` $\boldsymbol{p}$ `and add new boxes to` $\mathcal{L}$

Main data structures

- Two lists containing parts of the search space (boxes)
- Ordered working list $\mathcal{L}$
- Solution list $\mathcal{L}_{\text{final}}$

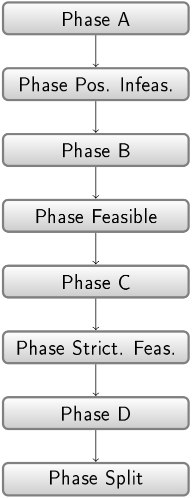
Termination criteria

- $\operatorname{wid} \boldsymbol{p} \leq \epsilon_p, \epsilon_p > 0$
- $\operatorname{wid}(\Phi(\boldsymbol{p})) \leq \epsilon_\Phi, \epsilon_\Phi > 0$

- Finds the minimum in the specified starting box
- Based on Hansen's interval optimization algorithm

Configurable Algorithm in UniVerMeC

Divided into phases



Configuration

Phase A
Midpoint Test

Phase Feasible
Update upper bound

Phase D
Linearization and pruning based on the consistency constraint

Phase Split
Calculate bound on $\Phi(\boldsymbol{p})$
Check for (in)consistent states

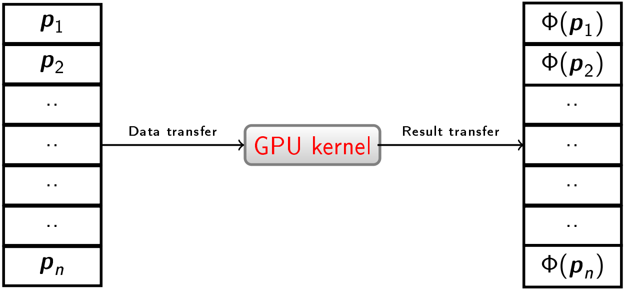
Use of GPU in Parameter Identification

$$\Phi(p) = \sum_{k=1}^{T} \left(y(t_k, p) - y_m(t_k)\right)^2$$

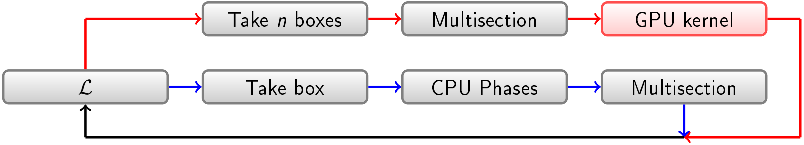
Value of $y(t_k, p)$ depends on $y(t_{k-1}, p)$

A single evaluation cannot be parallelized

But we can evaluate $\Phi(\boldsymbol{p})$ over different subdivision intervals in parallel!



Integration into the Optimization Algorithm



GPU and CPU run in parallel

Working list $\mathcal{L}$ is in host memory

One CPU thread feeds the GPU with data

Other CPU threads work normally

$\rightarrow$ Currently, only bounds on Φ are derived using the GPU

Quality Measure

Identified candidate intervals $\boldsymbol{p}$ are characterized by

$$e = \sqrt{\frac{\sum_{k=1}^{T} (y_{k-1} - y_m(t_k) + f(y_{k-1}, \mathrm{mid}(\boldsymbol{p})))^2}{T}} .$$

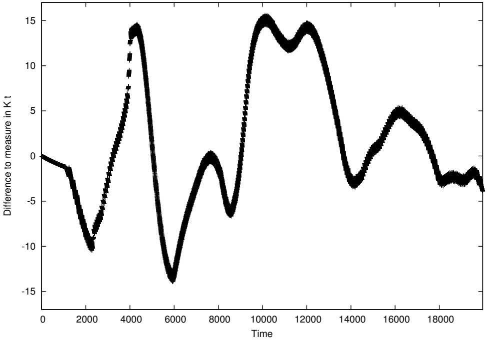
This measure is

- practice-motivated
- similar to the root mean square error measure

Candidate $\boldsymbol{p}$ with lowest e is chosen as solution, if there is no other way to proof that $\boldsymbol{p}$ is the optimum (minimum).

GPU Results ($1 \times 1 \times 1$)

Difference between measured and simulated temperature



	Error measure	Wall time
GPU	7.42944	$\approx 135s$
CPU (OpenMP)	7.68	$\approx 2491s$

Conclusions & Outlook

Conclusions

- An environment for SOFCs presented
- Flexibility wrt. different models and solvers implemented
- Model parameters identified by global optimization
- A speed up of 18 achieved for the $1 \times 1 \times 1$ model by GPU in the parameter identification algorithm (against the parallel CPU version)

Future Work

- Incorporate further solvers
- Allow easy addition of new models through a plugin based system
- Simulations for more complicated models

Thank You for Your Attention

Thank You for Your Attention!

References

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