DEALING WITH COMPLEX MODELS AND HOW TO USE THE IDEALIZATION OF PHYSICS TO OUR ADVANTAGE

Keynote at the 15th International Modelica Conference in Aachen Dr Dirk Zimmer, Institute of System Dynamics and Control 10.10.2023



What we regard as necessary:

A necessary condition is:

The equations whose solution represent a physical system can be distributed among its components



What we regard as necessary:



A necessary condition is:





What we may regard as sufficient:



A necessary condition is:

The equations whose solution represent a physical system can be distributed among its components

But more than that, we like to state a sufficient condition:

Any valid combination of components (under rules of limited complexity) shall have a solution representing a physical system.

What we may regard as sufficient:





Any valid combination of components (under rules of limited complexity) shall have a solution representing a physical system.

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What we may regard as sufficient:





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WHAT IS NECESSARY?

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A very simple Example to begin with...



 Going from the actual physical system to the mathematical model contains many, many implicit assumption that are hardly ever discussed...



Simulating the microverse:

- Maybe we can simulate the macroscopic system by applying the rules of quantum physics. Here we progress by a sum of quantum events (decoherences)

$$\sum_{k}^{k=t/t_{d}} |\psi\rangle_{k} \to |\phi_{i}\rangle_{k}$$

(arrow indicates a single event)

There is an estimation formula for the average time between such events for macroscopic systems:

$$t_d = t_R \ \frac{\hbar^2}{2mk_B T (\Delta x)^2}$$

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• Plugging in our parameters, yields for t = 10:

 $k = 10^{48}$

Why can we simulate macroscopic systems?

Fortunately, quantum physics fulfills the principle of stationary action:

 $\frac{\partial}{\partial q(t)} \int_{t_a}^{t_b} T(\dot{q}(t)) - V(q(t), \dot{q}(t)) dt = 0$





Why can we simulate macroscopic systems?

Fortunately, quantum physics fulfills the principle of stationary action:

$$\frac{\partial}{\partial q(t)} \int_{t_a}^{t_b} T(\dot{q}(t)) - V(q(t), \dot{q}(t)) dt =$$
Kinetic Energy Potential Energy Lagrangian: L

$$L(q, \dot{q}) = T - V$$
Action: S

$$S = \int_{t_a}^{t_b} L dt$$

* for the conservative case

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0

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Fortunately, quantum physics fulfills the principle of stationary action:

$$\frac{\partial}{\partial q(t)} \int_{t_a}^{t_b} T(\dot{q}(t)) - V(q(t), \dot{q}(t)) dt = 0^*$$
Kinetic Energy Potential Energy Lagrangian: L

$$L(q, \dot{q}) = T - V$$
Action: S

$$S = \int_{t_a}^{t_b} L dt$$

* for the conservative case



Can we solve this system reliably?

It is hard to make any statement about the potential energy:

$$\frac{\partial}{\partial q(t)} \int_{t_a}^{t_b} T(\dot{q}(t)) - V(q(t), \dot{q}(t)) dt = 0$$
Kinetic Energy Potential Energy

- In Modelica we mostly state the gradient of the potential energy. Hence, at least V is continuous.
- To illustrate the potential complexity, the example on the right is arbitrarily chosen.



Can we solve this system reliably?

Fortunately, kinetic energy has very beneficial properties:

$$\frac{\partial}{\partial q(t)} \int_{t_a}^{t_b} T(\dot{q}(t)) - V(q(t), \dot{q}(t)) dt = 0$$

Kinetic Energy



- It ensures continuity of q(t)
- It promotes locality of $\dot{q}(t)$
- It cannot be overpowered by V and is always inambiguous

The Kinetic Energy has a special role!

It is unlike all other forms of energy





Can we solve this system reliably?

-

Fortunately, kinetic energy has very beneficial properties:

$$\frac{\partial}{\partial q(t)} \int_{t_a}^{t_b} T(\dot{q}(t)) - V(q(t), \dot{q}(t)) dt = 0$$

Kinetic Energy

Potential Energy

The complexity of the action is growing over time for different straight paths. Solving is hence possible for small steps in $\Delta t = t_b - t_a$



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How do I solve principle of stationary action then?

The direct method is to apply the Euler-Lagrange equations:

$$\frac{\partial}{\partial q(t)} \int_{t_a}^{t_b} T(\dot{q}(t)) - V(q(t), \dot{q}(t)) dt = 0$$
Kinetic Energy Potential Energy Lagrangian: L

$$L(q, \dot{q}) = T - V$$

 Unfortunately, the Lagrangian view results in a solution that cannot be distributed among its components. $\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = 0$





Fortunately, Sir William Hamilton created another formulation that doubles the (resulting) dimension :

 $L(q,\dot{q}) \rightarrow H(q,p)$

• ... by introducing the generalized potential:

$$b_i = \frac{\partial L}{\partial \dot{q}^i}$$

The Hamiltonian is then expresses the total energy*:

$$H = T + V$$

* under certain conditions







This leads to a reformulation of the action and a solution based on the Hamiltonian:



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Let us go through one example: The pressure wave in a pipe

- Our path is expressed by the integral of volume flow: q(t) = Q
- Hence also: $\dot{q}(t) = \dot{Q}$
- Which means for the kinetic energy: $T = \frac{I\rho}{2}\dot{Q}^2$ (with $I = \int \frac{ds}{A}$)
- The potential energy is: $V = \frac{K}{2Q_{ref}} Q^2$ (if Q and Q_{ref} are close and fluid incompressible)



• The Lagrangian
$$L = \frac{I\rho}{2}\dot{Q}^2 - \frac{K}{2Q_{ref}}Q^2$$

• Now for
$$p = \frac{\partial L}{\partial \dot{q}} = \frac{\partial (\frac{I\rho}{2}\dot{Q}^2 - \frac{K}{2Q_{ref}}Q^2)}{\partial \dot{Q}} = I\rho\dot{Q}$$

• Then: $H = \frac{1}{2}\frac{p^2}{I\rho} + \frac{K}{2Q_{ref}}Q^2$

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• Hamiltonian:
$$H = \frac{1}{2I\rho}p^2 + \frac{K}{2Q_{ref}}Q^2$$

Plugging this into the Hamiltonian equation yields:



Harmonic Oscillation



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• Hamiltonian:
$$H = \frac{1}{2I\rho}p^2 + \frac{K}{2Q_{ref}}Q^2$$

Plugging this into the Hamiltonian equation yields:





$$\begin{split} \ddot{Q}I\rho &= \frac{dp}{dt} \\ \frac{dp}{dt} &= -\frac{K}{Q_{ref}}Q \end{split}$$

- It may help to define the pressure $P = \frac{dp}{dt}$
- This form may now be distributed.

$$\frac{d\dot{\boldsymbol{Q}}}{dt}I\rho = \boldsymbol{P}$$

$$\frac{d\boldsymbol{P}}{dt}\frac{Q_{ref}}{K} = -\dot{\boldsymbol{Q}}$$



The pairs of Potential and Flow



The equations are distributed to components:

•
$$\frac{d\dot{Q}}{dt}I\rho = \Delta P$$

•
$$\frac{d\mathbf{P}}{dt}\frac{Q_{ref}}{K} = -\dot{\mathbf{Q}}$$

- The doubling of the resulting dimensions by H created our beloved pairs of potential and flow:
 - dp/dt, here Pressure **P**
 - q or sometimes dq/dt as here with the Volume flow Q



Modeling Additional Components



The equations are distributed to components

•
$$\frac{d\dot{\mathbf{Q}}}{dt}I\rho = \Delta P$$

$$\frac{d\mathbf{P}}{dt}\frac{Q_{ref}}{K} = -\dot{\mathbf{Q}}$$

Using this pair, we can model further components:

•
$$\zeta \frac{\dot{\boldsymbol{Q}} |\dot{\boldsymbol{Q}}|}{\dot{Q}_{ref}^2} = \Delta \boldsymbol{P}$$

$$\frac{d\mathbf{P}}{dt}\frac{A}{\rho g} = -\dot{\mathbf{Q}}$$

Composing the complete system



• Finally we can simulate the complete system



Modeling is a lossy compression of reality



Quantum Events	ODE Approach	
$\sum_{k}^{k=t/t_{d}} \psi\rangle_{k} \to \phi_{i}\rangle_{k}$	$\mathbf{x}_t = \mathbf{x}_0 + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1})$	
$k > 10^{48}$ $\underline{\eta} >$	$k = 5 \cdot 10^7$ $\dim(\mathbf{x}) = 9$	

- Principle of stationary action
- Law of large numbers
- Homogeneity Assumptions
- Discretization of Space
- Continuity Assumption
- Floating Point Approximation
- Discretization of Time

•

Recapitulation



- The principle of stationary is the basis for classic physics
- The presence of kinetic energy ensures solvability of this principle
 - Being based on the derivative q̇, ensures continuity.
 - Its quadratic nature promotes locality of the solution
 - Having a bijective and unbounded gradient field means that the kinetic energy can never be overpowered.
- The Hamiltonian view (q, q) → (q, p) doubles the resulting dimension and enables the distribution of the equations and gives rise to the pairs of effort and flow for the components interface.

S =L dt $L(q,\dot{q}) \rightarrow H(q,p)$

Recombining the result

There is an easy way to improve efficiency. Let us simply forget about modeling the pipe:





Recombining the result

There is an easy way to improve efficiency. Let us simply forget about modeling the pipe:





Recombining the result



- This is extremely effective. We are much faster now.
- But beware, we now have a non-linear equation system to solve:
 - The pressure level below the valves needs to balance out the flows.



Modeling is a lossy compression of reality



Quantum Events	ODE Approach	DAE Approach		
$\sum_{k}^{k=t/t_{d}} \psi\rangle_{k} \to \phi_{i}\rangle_{k}$	$\mathbf{x}_t = \mathbf{x}_0 + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1})$	$\mathbf{x}_{t} = \mathbf{x}_{0} + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1}, \mathbf{s}_{k,i})$ $\mathbf{s}_{k,i} \in \{\mathbf{s}_{k} 0 = g_{k}(\mathbf{s}_{k})\}$		
$k > 10^{48}$ $\frac{\eta > 10^{10}}{100}$	$k = 5 \cdot 10^7$ dim(x) = 9 $\underline{10^{40}}$	$k = 10^{1}$ $\dim(\mathbf{x}) = 3$ $\dim(\mathbf{s}) = 1$		
Principle of	stationary action			
• Law of larg	e numbers			
Homogene	ity Assumptions			
Discretization	on of Space			
Continuity A Floating Po	int Approximation			
Discretizati	on of Time			
•				

What can we say about the solvability?

Can we make a general statement about the solvability?

$$\frac{\partial}{\partial q(t)} \int_{t_a}^{t_b} \frac{1}{V(q(t), \dot{q}(t))} dt = 0$$
Kinetic Energy Potential Energy

- The new system does not contain any model for the kinetic energy anymore.
- We have removed exactly the part that helped to ensure solvability.
- There is actually not a meaningful Lagrangian anymore!
 Does this still represent a physical system?

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Practical Application Example 1: Inertia of Turbine Shaft





- This thermodynamic process yields a non-linear system that can be very difficult to solve.
- We need to find the power balance between compressor, fan and turbine
- Adding an inertia to the shaft connecting turbine and compressor helps enormously

Practical Application Example 2: Constrained Mechanics





Practical Application Example 2: Constrained Mechanics

- At the point of maximum extension the kinetic energy is constrained.
- The kinetic energy cannot be transferred since all bodies are assumed to be rigid.
- Elasticity needs to be added

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Preliminary Conclusions



- To ensure solvability, kinetic energy plays a vital role
- The Hamiltonian Form which is the basis for our standard interfaces is indifferent to kinetic energy and may mislead us.

n dimensional result $L(q, \dot{q}) = T - V$ kinetic energy is special 2n dimensional result H(q,p) = T + Vkinetic energy is one among many

The Hamiltonian offers a very general expression for the conservation of total energy but it is the action that tells us how to solve the system.



WHAT IS SUFFICIENT?

Modeling is a lossy compression of reality



Quantum Events	ODE Approach	DAE Approach		
$\sum_{k}^{k=t/t_{d}} \psi\rangle_{k} \to \phi_{i}\rangle_{k}$	$\mathbf{x}_t = \mathbf{x}_0 + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1})$	$\mathbf{x}_{t} = \mathbf{x}_{0} + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1}, \mathbf{s}_{k,i})$ $\mathbf{s}_{k,i} \in \{\mathbf{s}_{k} 0 = g_{k}(\mathbf{s}_{k})\}$		
$k > 10^{47}$ $\underline{\eta > }$	$k = 5 \cdot 10^{7}$ dim(x) = 9 $\underline{10^{40}}$	$k = 10^{1}$ $\dim(\mathbf{x}) = 3$ $\dim(\mathbf{s}) = 1$		
Principle of	extremal action			
 Law of large Homogene Discretization Continuity / Floating Point Discretization 	e numbers ity Assumptions on of Space Assumption int Approximation on of Time	2		

Modeling is a lossy compression of reality



Quantum Events	ODE Approach	DAE Approach		
$\sum_{k}^{k=t/t_{d}} \psi\rangle_{k} \to \phi_{i}\rangle_{k}$	$\mathbf{x}_t = \mathbf{x}_0 + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1})$	$\mathbf{x}_{t} = \mathbf{x}_{0} + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1}, \mathbf{s}_{k,i})$ $\mathbf{s}_{k,i} \in \{\mathbf{s}_{k} 0 = g_{k}(\mathbf{s}_{k})\}$		
$k > 10^{47}$ $\underline{\eta >}$	$k = 5 \cdot 10^7$ dim(x) = 9 $\eta > \eta$	$k = 10^{1}$ $\dim(\mathbf{x}) = 3$ $\dim(\mathbf{s}) = 1$		
• Principle of	f extremal action • Simul	taneity		
 Law of larg Homogene Discretizati Continuity Floating Po 	e numbers Instar ity Assumptions Conse on of Space Assumption int Approximation	ntaneity ervation laws		
 Discretizati 	on of lime			

About Simultaneity.

- <u>Simultaneity</u> is a non-physical concept.
 It wrongfully assumes the existence of a global time
- However, our computing devices have their own clock Simultaneity is thereby a very powerful concession; pleasing the way we compute.
- In our example we could gain a factor of 10⁷ by replacing propagation of energy through a wave by the direct <u>instantaneous</u> transfer of energy between potentials.
- It is a powerful but a little dangerous concept







Making different Use of Simultaneity



But here is another way to achieve the result:



And the efficiency is almost as good as working with the potentials

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Modeling is a lossy compression of reality



ODE Approach	LIED Approach	DAE Approach		
$\mathbf{x}_t = \mathbf{x}_0 + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1})$	$\mathbf{x}_{t} = \mathbf{x}_{0} + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1}, \mathbf{s}_{k})$ $\mathbf{A}_{k}\mathbf{s}_{k} = \mathbf{b}_{k}$	$\mathbf{x}_{t} = \mathbf{x}_{0} + \sum_{k=1}^{k=t/h} hf(\mathbf{x}_{k-1}, \mathbf{s}_{k,i})$ $\mathbf{s}_{k,i} \in \{\mathbf{s}_{k} 0 = g_{k}(\mathbf{s}_{k})\}$		
$k = 5 \cdot 10^7$ $\dim(\mathbf{x}) = 9$ $\underline{\eta} >$	$k = 1 \cdot 10^{1}$ dim(x) = 5 dim(s) = 2 $\underline{\eta}$	$k = 10^{1}$ $\dim(\mathbf{x}) = 3$ $\dim(\mathbf{s}) = 1$		
 Simu kinet Instate 	taneity on • Simul ic energy poten ntaneity • Conse	taneity on tial energy ervation laws		

Making different Use of Simultaneity

One idea to get the best of both worlds:

- Let us apply the concept of simultaneity but
 - avoid the direct exchange of potential energy
 - instead just apply it to kinetic energy.
- To implement this, we need to re-establish the special role of kinetic energy in our connector:
 - This needs another dimension and we have to split up the potential variable:
 - For hydraulics: we decompose the pressure:

 $p = \hat{p} + r$

with r being the inertial pressure resulting from the kinetic energy of the flow.





Implementation in DLR ThermoFluid Stream / HEXHEX

- For a general solution, we need a special interface
 - The pair (r, m) represents the kinetic part and builds up a linear equation systems
 - The signal Θ represents the thermodynamic state based on $\hat{p} = p r$
- With a partial base model we ensure that the kinetic energy is always present.
- We can then choose to either directly couple the kinetic parts or whether they shall interact with the potentials (boundaries, volumes). We thereby limit the spatial frequency of interaction.





Implementation in DLR ThermoFluid Stream / HEXHEX





- All components take kinetic energy into account.
- The connector enables us to use one state for each branch of mass-flow rate
- The connector enables us to limit the choose a different spatial resolution for r than for p̂.



Robust component models

Robust system model

This method scales...



This method scales...





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This method scales...





- The ENERGIZE model describes a more electric aircraft with 220 passengers
- Combination of thermal and electrical power management.
- Complete aircraft missions through different environmental conditions can be simulated.
- > 18,000 Equations
- > 300 States

Implementation in Dialectic Mechanics

In Mechanics we can go for a similar solution:

- The pair v_{kin} , f cares about the kinetic energy
- The position signal r describes the current configuration
- Again we can ensure the presence of kinetic energy in all dimensions
- We can limit the temporal interaction frequency between elastic potentials and kinetic energy at the joint elements by stating

•
$$\frac{dv_{kin}}{dt} T_D = \frac{dr}{dt} - v_{kin}$$

```
connector Flange
[...]
SI.Velocity v_kin;
flow SI.Force f;
input SI.Position r;
```

end Inlet;



Implementation in Dialectic Mechanics





- With only linear equations and bounded eigenvalues, Dialectic Mechanics is very attractive for real-time applications
- Gripping
- Variable Structure Systems
- Even stiff system can be computed in hard real-time.

Linear Implicit Equilibrium Dynamics

The way of modeling that we derived leads to a special class of DAE systems: Linear Implicit Equilibrium Dynamics.

$$0 = F(\mathbf{x}_P, \dot{\mathbf{x}}_P, \mathbf{u}, t)$$

$$\dot{\mathbf{x}}_N = f(\mathbf{x}_L, \mathbf{x}_N, \mathbf{u}, t)$$

$$\dot{\mathbf{x}}_N = f(\mathbf{x}_L, \mathbf{x}_N, \mathbf{u}, t)$$

...where g and f can be constructed just by sorting the equations of F. Given $\mathbf{x}_L \cup \mathbf{x}_N = \mathbf{x}_P$ with $\mathbf{x}_L \cap \mathbf{x}_N = \{\}$

- Hence the implicit part may only expressed using the matrix L
- What looks like a very restrictive class of models is actually more powerful than what we might think.

Linear Implicit Equilibrium Dynamics and Pre-Compilation



- It turns out that pre-compilation of Components is feasible for LIED systems.
- A component then yields several blocks of code:

```
model PressureDrop
TFSPlug inlet;
TFSPlug outlet;
parameter VolumeFlowRate v_ref;
parameter Pressure dp_ref;
VolumeFlowRate v_norm;
SI.Pressure dp;
SI.MassFlowRate m;
equation
v=inlet.m.flow/rho(inlet.state);
v_norm = v/v_ref;
dp*2 = dp_ref*(v_norm+v_norm^2);
inlet.m + outlet.m = 0;
v = inlet.v;
inlet.p - dp = outlet.p;
```

end PipeFrictionNL;

```
void PressureDrop::evalState() {
  const double v = inlet.m.flow/rho(inlet.state);
  const double v_norm = v/v_ref;
  const double dp = 0.5*dp_ref*(v_norm + v_norm*v_norm);
  outlet.state.h = inlet.state.h;
  outlet.state.p = inlet.state.p - dp;
```

void PressureDrop::evalFlow() {outlet.m = -inlet.m;}

Variable Structure Systems

- For LIED systems, the code blocks would then be sorted. This can be done at run-time.
 - In our example:
 - evalState() and
 evalFlow() are both sorted
 downstream
 - evalInertia() is sorted upstream.
- Then Variable Structure Systems suddenly become quite trivial





CONCLUSIONS



From Necessary to Sufficient

 Our current standard interfaces, ultimately result from Hamilton's trick to double the dimension. They are what is <u>necessary</u> for object-oriented modeling.

Domain	Translational Mechanics	Rotational Mechanics	Hydraulics	Electrics	Thermal	
Potential	r	arphi	Р	V	Т	
Flow	f	τ	Ż	i	Q	



 We can find extended interfaces that offer a <u>sufficient</u> form. (Unfortunately hardly anyone is looking for these forms)

Domain	Translational Mechanics	Rotational Mechanics	Thermo Fluids	Electrics	?	
Potential	v_{kin}	ω_{kin}	r	?		
Flow	f	τ	'n	?		
Signal	r	arphi	Θ	?		

The Value of a Sufficient Statement



- Sufficient forms have rules for their components and their composition.
- ThermofluidStream
 A
 - ~ 🚺 User's Guide
 - Basic composition rules
 - Nomenclature
 - Release notes

Important Claim/Observation:

The complexity of these rules transfers to the complexity of code generation

- This is the key to pre-compilation, variable structure system, large systems etc.
- LIED Systems are one primary example.

A Dire Word of Warning



Insisting on solutions that work on arbitrary general hybrid non-linear DAE Systems is a sure way to stall progress...



Source: Homer the Great, The Simpsons, TV Series S6 Ep12

... it did so the last 20 years and will do so in the next 20 years.

• We should simple be pragmatic and support forms that have a rule set.

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On Our Future



- Our libraries of free and commercial models is our biggest asset.
- We form a wonderful community hosting and nurturing these models.
- We should support models of all kind. Those who profit from rules and those who want freedom.
- Sufficient forms may spur progress in many areas!
- The upcoming AI Revolution will swipe over everything that is high-level.

Having a good understanding of the low-level is what will make us thrive and survive.

References to current work on sufficient forms



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