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Leibniz Institute for Information Infrastructure

The publication-based approach for mathematical models: Identification of mathematical models

Wolfram Sperber

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RISC, Hagenberg
2018-08-13

INTRODUCTION

AN EXAMPLE

THE PUBLICATION-BASED APPROACH

MODEL INFORMATION IN PUBLICATIONS

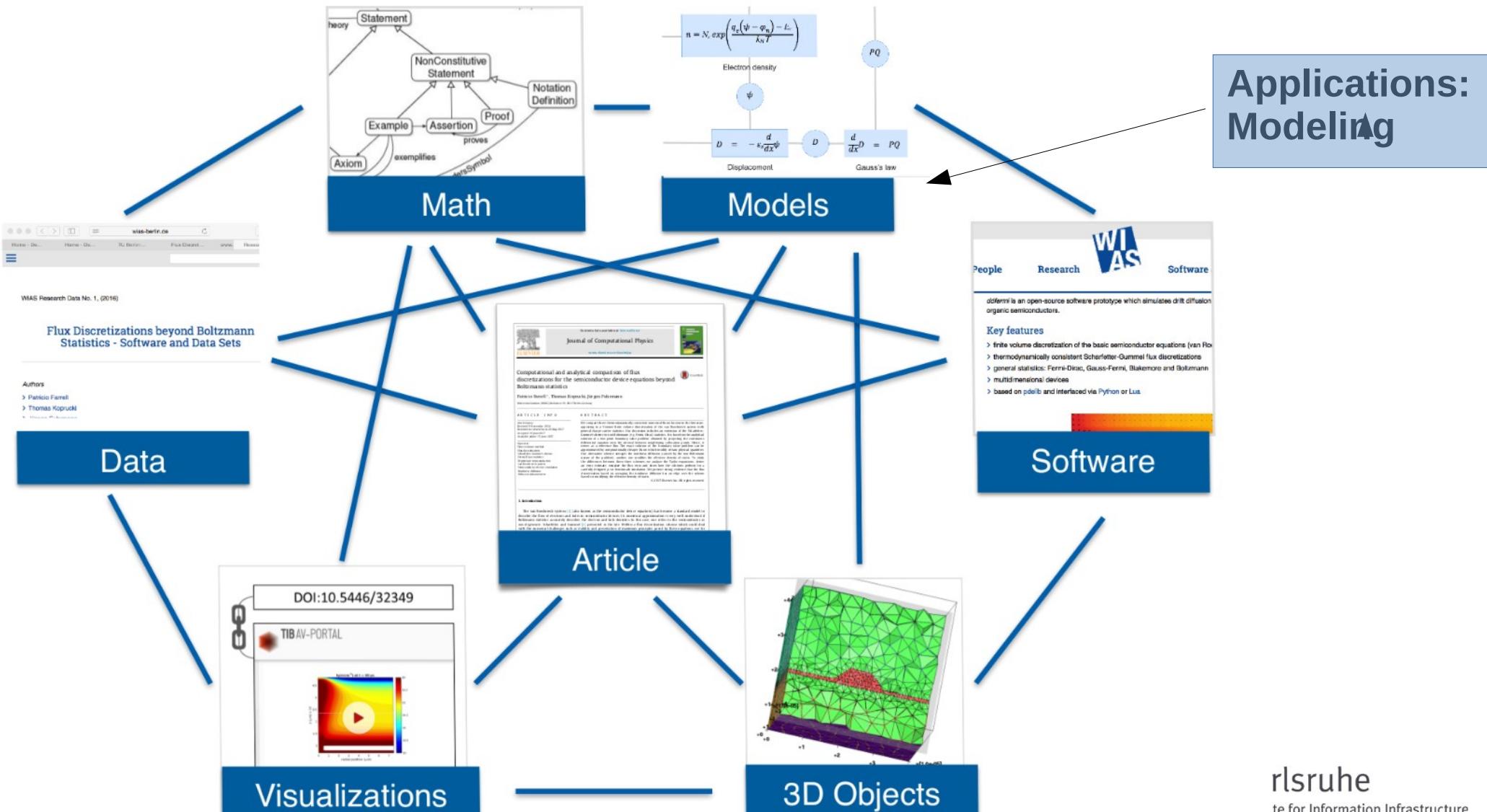
THE MODEL TENSOR

OUTLOOK



The central role of mathematical models

A slide
of Thomas



The goal and the idea

Building up a useful service for mathematical models:

- Thomas/Michael: Models play a central role for mathematical research
- How can we build a useful service for mathematical models?

The problem

- Typically, up to now models are part of publications and not marked as single objects

Difficulties with mathematical models

“Mathematical model” is not a exactly defined term. Mathematical models can be formulated in a real-world context (an increasing number of mathematical models has a non-mathematical background) or context-free.

- Mathematical models are given by definitions, only a small number of models has also a name.
- More pragmatic:
The definitions of mathematical models in many publications are incomplete.

Challenges for the publication-based approach

- Identification of mathematical models in publications and the analysis of the information about models is closely related:
Definitions contain specific content information.

Technically:

- In general, the definitions of the mathematical model which is investigated is given in the fulltexts of publications, not in the review or abstract.
- Mathematical definitions contain mathematical expressions (symbols, formulae) plus text. Therefore we need more than the fulltext in PDF format.
At least TeX-encoded sources of the publications are necessary.
arXiv seems to be a first resource.

A first approach

- 1) Where can we find information about mathematical models?
→ analysis of the document structure
- 2) How can we extract and analyze information about mathematical models?
Which information about mathematical models is possible?
→ weak description model for mathematical models

Hybrid quantum-classical modeling of quantum dot devices

Markus Kantner^{*} Markus Mittnenzweig, and Thomas Koprucki

Weierstrass Institute for Applied Analysis and Stochastics,
Mohrenstr. 39, 10117 Berlin, Germany

The structure (TOC):

- I. Introduction
- II. Model equations
 - A. Van Roosbroeck System
 - B: Quantum master equation
 - C. Macroscopic coupling terms and charge conservation
- III. Thermodynamics
 - A. Energy, charge, and entropy balance
 - B. Thermodynamic equilibrium
 - C. Microscopic transition rates and the quantum detailed balance condition
- IV. Application to electrically driven single-photon sources
 - A. Model specification
 - B. Numerical simulation method
 - C. Device specification
 - D. Stationary operation
 - E. Pulsed operation
- V. Discussion and Outlook
- VI. Summary
 - plus Acknowledgments and Appendices A-F

Hybrid quantum-classical modeling of quantum dot devices

Markus Kantner^{*} Markus Mittnenzweig, and Thomas Koprucki

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For humans:

In Title: Modeling

in Abstract: modeling: 'By coupling the van Roosbroeck equation with a quantum master equation in
Lindblad form, ...'

in Introduction: → Model Equations in Sec. II

$$-\nabla \cdot \varepsilon \nabla \psi = q (p - n + C + Q(\rho)), \quad (1)$$

$$\partial_t n - \frac{1}{q} \nabla \cdot \mathbf{j}_n = -R - S_n(\rho; n, p, \psi), \quad (2)$$

$$\partial_t p + \frac{1}{q} \nabla \cdot \mathbf{j}_p = -R - S_p(\rho; n, p, \psi), \quad (3)$$

$$\frac{d}{dt} \rho = \mathcal{L}(\rho; n, p, \psi) = -\frac{i}{\hbar} [H, \rho] + \mathcal{D}(\rho; n, p, \psi) \quad (4)$$

on the domain $\Omega \subset \mathbb{R}^3$. The system (1)–(4) is subject to initial conditions and boundary conditions modeling electrical contacts and other interfaces [32]. See Appendix A

→ Model Consistency III
→ Application

What is the model in the paper?

in textual form:

'hybrid quantum-classical model that self-consistently couples semi-classical transport theory to a kinetic equation for the quantum mechanical density matrix.'

as mathematical expressions (equations):

$$-\nabla \cdot \varepsilon \nabla \psi = q(p - n + C + Q(\rho)), \quad (1)$$

$$\partial_t n - \frac{1}{q} \nabla \cdot \mathbf{j}_n = -R - S_n(\rho; n, p, \psi), \quad (2)$$

$$\partial_t p + \frac{1}{q} \nabla \cdot \mathbf{j}_p = -R - S_p(\rho; n, p, \psi), \quad (3)$$

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on the domain $\Omega \subset \mathbb{R}^3$. The system (1)–(4) is subject to initial conditions and boundary conditions modeling electrical contacts and other interfaces [32]. See Appendix A

But

- the model is incomplete: (1)-(4) are the partial differential equations. They must be completed by initial- and boundary equations
→appendix (This is trivial for the mathematicians.)
- the model is specified (some hypotheses for the application case):
 - (1)-(4) are the basic equations
 - (1)-(3) van Roosbroeck (semi-classical transport model for electrons and holes)
 - (4) quantum master equation
- there are additional equations and principles which are presented in the subsection A, B, C and section III (evaluation of modeling: correctness accordance with the principles of thermodynamics).
- *Remark: This paper describes the modeling process (the model is the result of this paper), not the mathematical treatment of the model.*

A first summary

- The model is given by text and formulae.

For the mathematical treatment the formulae are the most important part. Often the textual environment gives some information about the meaning of the expression and the background of the model (origin / use cases) but can contain also structural information as in the example (van Roosbroeck, quantum master equation in Lindblad form, links to scientific theories, algorithms, software, ...)

- Both the textual information and the mathematical expressions which describe a model are relevant.
- Therefore we should try to extract both
 - the mathematical expressions describing the model
 - the corresponding terms and phrases for the mathematical expressions
- *Remark: Terms, phrases and mathematical expressions are ambiguous, but mathematical expressions, especially complex objects as equations, inequalities, structural diagrams contain precise information about their structure which allow to compare these objects and enhanced retrieval features.*

What can we do automatically?

- **The publication-based approach for mathematical models**

Up to now, models are part of publications. →Therefore we have to develop methods to extract the

- mathematical expressions describing the mathematical model and the corresponding terms and
- phrases.

Remarks:

- **Fulltexts:**

The most abstracts or reviews, the zbMATH data, don't contain precise model descriptions.

Typically, the mathematical expressions are not part of the abstract or reviews. Therefore, we need the fulltexts of the models.

- **Formats:**

Up to now, no powerful converter exists for transforming PDF formatted documents to TeX or MathML. At least, TeX encoded documents are needed. Therefore the arXiv e-prints are a first resource to develop methods for model analysis.

The publication-based approach

The publication-based approach covers three steps:

1) Identification of the model-relevant parts of the publication

- Model relevant sections or subsections

which can be identified by characteristic terms in the titles, especially 'model*' or
'problem*'

alternatively

- the beginning of a document, e.g., the first 3,000 characters

A statistic

Journal	(Sub-)sections containg the terms `model' or `problem'
International Journal of Robust and Nonlinear Control, v. 10, n. 28	8 (9)
International Journal of Robust and Nonlinear Control v. 10, n. 29	6 (8)
Journal of System Science & Complexity v. 31, n. 3	7 (13)
Cybernetics and System Analysis v. 54, n. 2	8 (18)
International Journal of Control and Signal Processing v. 32, n. 6	7 (10)
Automation and Remote Control, v. 79, n. 5	6 (12)

Identification of model-relevant parts: results and open questions

by eliminating the non-relevant parts we get reduced (TeX-encoded) artifacts which contain only the model-relevant parts

- *Remark: It is not clear that the model-relevant parts contain only one model information. The reduced document can also contain previous models, similar models, specific models, generalized models, transformed models, etc.). In other words, it may contain a lot of additional information. How can we eliminate redundant / irrelevant information? (If yes, we could markup the model in the original file by a 'model tag')*

Our example: The section II contains ~ 100 mathematical expressions
9 / A:22 / B:29 / C:18 / fig.2:(15) text:10) (moreover, the mathematical expression from appendix A must be added).
The frequencies of some expressions is > 1.

Analysis of the model-reduced documents

2) Analysis of our artifacts:

- 1) extraction of all mathematical expressions (TeX or MathML encoded expressions)
and the corresponding terms and phrases
→ creating a ‘model-related’ matrix A_{i3} ($1 \leq i \leq n$, n – number of mathematical expression in the model-reduced document) for a document with the components :

a_{i1} : mathematical expression

a_{i2} : left-hand textual neighborhood (k terms)

a_{i3} : right-hand textual neighborhood (k terms)

Example: C	doping profile	0
Q(p)	expectation value of the charge density	0
n	free electron density	0
p	free hole density	0
(1)-(3)	0	van Roosbroeck system

Analysis of the model-reduced documents: results and open questions

storing in a database ($A_{i_3}^k$ with k as the number of k -th document)

Remarks: As result we get a tensor which contains mathematical expressions plus their neighborhood. The mathematical expressions are listed in the sequence of their occurrence. This can make difficulties, e.g., parts of the model are presented at different positions in the document.

Can we identify the input variables of the model?

How can we organize it in a better way (sorting by length is not a real good idea)?

How can we identify the system structure of a model?

How can we find relevant textual information for a mathematical expression which is not in the left- or in the right-hand neighborhood of a mathematical expression?

What do we do with this information (e.g, storing this information in a special field of the tensor)?

Further processing: Transformation of the TeX-encoded mathematical expressions

3) It is difficult to compare TeX-encoded mathematical expressions
(the TeX codes for a PDF document differ; zbMATH experience: mathematical expressions with more than 6 characters occur in the database zbMATH only once)
better (more standardized): XML / MathML encoded mathematical expression
(tree structured documents)
MathML transformation of mathematical expressions via **LaTeXML**
→ tree-structured documents which allow to compare the structure of mathematical formulae

*Remarks: LaTeXML transform the TeX code to XML. By postprocessing, the XML code can be transformed to MathML (Presentation Markup, Content Markup, or OpenMATH)
Which format should be used for storing, all or only MathML Content Markup?
(If the authors would write their documents in STeX, MathML or OpenMATH should be used).*

Example (the PDE system 1 - 4)

```
\begin{align}
-\nabla\cdot\nabla\psi &= q(\rho - n + C + Q), \\
\text{label}{eq: Poisson equation}\\
\partial_t n - \frac{1}{q} \nabla\cdot(\mathbf{j}_n) &= -R_S(n)(\rho; n, p, \psi), \\
\text{label}{eq: electron transport}\\
\partial_t p + \frac{1}{q} \nabla\cdot(\mathbf{j}_p) &= -R_S(p)(\rho; n, p, \psi), \\
\text{label}{eq: hole transport}\\
\frac{d}{dt}\rho = \mathcal{L}(\rho; n, p, \psi) &= -\frac{i}{\hbar}(H\rho + \mathcal{D}\rho), \\
\text{label}{eq: quantum master equation}
\end{align}
```

The Online Editor of LaTeXML



ItxMojo: LaTeXML's Web Server

No obvious problems (Details)

```
1 \begin{aligned} 2 -\nabla\cdot\nabla\psi &= q\left(p-n+C+Q\right) \\ 3 \partial_t n - \frac{1}{q}\nabla\cdot\mathbf{j}_n &= -R - S_n(p, n, p, \psi), \text{ eq: Poisson equation} \\ 4 \partial_t p + \frac{1}{q}\nabla\cdot\mathbf{j}_p &= -R - S_p(p, n, p, \psi), \text{ eq: hole transport} \\ 5 \frac{\partial}{\partial t}(\rho) - \mathcal{L}(\rho, n, p, \psi) &= -\frac{i}{\hbar}[\mathcal{H}, \rho] + \mathcal{D}(\rho, n, p, \psi), \text{ eq: quantum master equation} \\ 6 \end{aligned}
```

[About](#)[Upload & Convert](#)[Web Editor](#)[Help](#)

On-the-Fly Preview

$$-\nabla \cdot \varepsilon \nabla \psi = q(p - n + C + Q(\rho)), \quad (1)$$

$$\partial_t n - \frac{1}{q} \nabla \cdot \mathbf{j}_n = -R - S_n(\rho; n, p, \psi), \quad (2)$$

$$\partial_t p + \frac{1}{q} \nabla \cdot \mathbf{j}_p = -R - S_p(\rho; n, p, \psi), \quad (3)$$

$$\frac{d}{dt} \rho = \mathcal{L}(\rho; n, p, \psi) = -\frac{i}{\hbar} [H, \rho] + \mathcal{D}(\rho; n, p, \psi) \quad (4)$$

</bref></cite>. The model equations read</p>
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</XMApp>
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</XMWrap>
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Some remarks and questions

All mathematical expressions of our model description tensor could be transformed on this way to MathML PM or CM or OpenMATH. This allows to use graph-based models, e.g. for comparing models or retrieval.

➤ **The advantage of the approach:**

All steps of the publication-based approach can be done widely automatically.

But the method has also some disadvantages:

In principle our model tensors of publications should contain the model information, but it is possible that the information is too much. How can we remove model-irrelevant information?

Big tensors describing a model are not very impressive for the user. How can we compactify the model representations

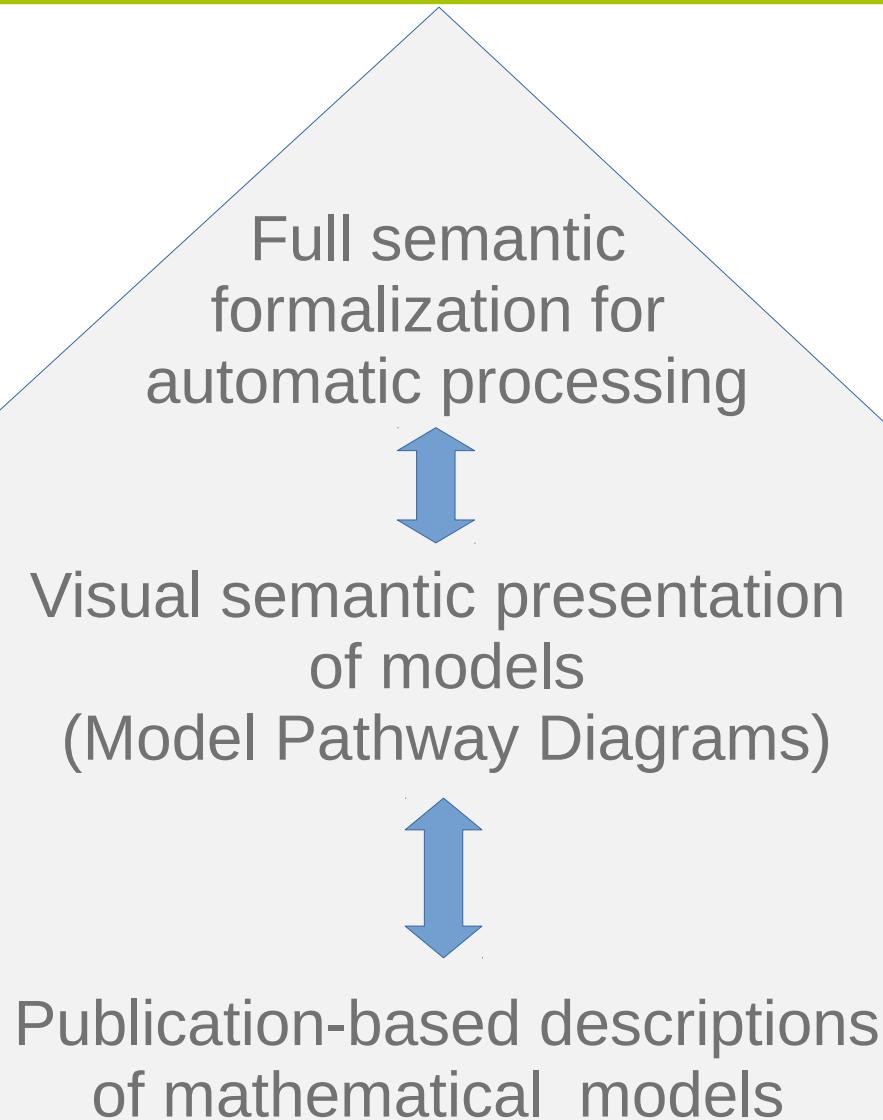
(A first idea:

A grouping of complex mathematical expressions with the involved notations should be possible. Often long mathematical expression are complex expressions (especially PDEs) containing special symbols which we could connect).

Further questions

- What is with retrieval (access for mathematicians and for non-mathematicians)?
- How can we detect similar models (ranking of the mathematical expressions of the models)?
- How can we make the service interactive (for improving the model, linking to further model information)?
- How can we make the modeling process understandable?

Our ambitioned goal: Building up a knowledge base for mathematical models



1. INTRODUCTION

In this paper, we consider a system of N spherical particles $(B_i)_{1 \leq i \leq N}$ with identical radii R immersed in a viscous fluid satisfying the following Stokes equation:

$$(1) \quad \begin{cases} -\Delta u^N + \nabla p^N &= 0, \\ \operatorname{div} u^N &= 0, \end{cases} \quad \text{on } \mathbb{R}^3 \setminus \bigcup_{i=1}^N \overline{B_i},$$

completed with the no-slip boundary conditions:

$$(2) \quad \begin{cases} u^N &= V_i + \Omega_i \times (x - x_i), \\ \lim_{|x| \rightarrow \infty} |u^N(x)| &= 0, \end{cases} \quad \text{on } \partial B_i,$$

where $(V_i, \Omega_i) \in \mathbb{R}^3 \times \mathbb{R}^3$, $1 \leq i \leq N$ represent the linear and angular velocities,

$$B_i := B(x_i, R).$$

We describe the inertialess motion of the rigid spheres $(B_i)_{1 \leq i \leq N}$ by adding to the instantaneous Stokes equation the classical Newton dynamics for the particles $(x_i)_{1 \leq i \leq N}$:

$$(3) \quad \begin{cases} \dot{x}_i &= V_i, \\ F_i + mg &= 0, \\ T_i &= 0, \end{cases}$$

where m denotes the mass of the identical particles adjusted for buoyancy, g the gravitational acceleration, F_i (resp. T_i) the drag force (resp. the torque) applied by the the fluid

¹

**Example 2:
The model
description
in the e-print
arXiv:1806.07795**

on the i^{th} particle B_i defined as

$$\begin{aligned} F_i &:= \int_{\partial B_i} \sigma(u^N, p^N) n, \\ T_i &= \int_{\partial B_i} (x - x_i) \times [\sigma(u^N, p^N) n], \end{aligned}$$

with n the unit outer normal to ∂B_i and $\sigma(u^N, p^N) = 2D(u^N) - p^N \mathbb{I}$, the stress tensor where $2D(u^N) = \nabla u^N + \nabla u^{N\top}$.

The publicly available TeX-code

```
\section{Introduction}
In this paper, we consider a system of  $(B_i)_{1 \leq i \leq N}$  spherical particles with identical radii  $R$  immersed in a viscous fluid satisfying the following Stokes equation:
\begin{equation}\label{eq_stokes}
\left. \begin{array}{l}
-\Delta u^N + \nabla p^N = 0, \\
\operatorname{div} u^N = 0,
\end{array} \right. \text{on } \mathbb{R}^3 \setminus \underbrace{\overline{\bigcup_{i=1}^N B_i}}_{\text{the domain}}
\end{equation}
completed with the no-slip boundary conditions:
\begin{equation}\label{cab_stokes}
\left. \begin{array}{l}
u^N = V_i + \Omega_i \times (x - x_i), \text{ on } \partial B_i, \\
|u^N(x)| = 0,
\end{array} \right. \text{as } |x| \rightarrow \infty
\end{equation}
where  $(V_i, \Omega_i) \in \mathbb{R}^3 \times \mathbb{R}^3$ ,  $1 \leq i \leq N$  represent the linear and angular velocities.
\begin{eqnarray*}
B_i &:=& B(x_i, R).
\end{eqnarray*}
We describe the inertialess motion of the rigid spheres  $(B_i)_{1 \leq i \leq N}$  by adding to the instantaneous Stokes equation the classical Newton dynamics for the particles  $(x_i)_{1 \leq i \leq N}$ :
\begin{equation}\label{ode}
\left. \begin{array}{l}
\dot{x}_i = V_i, \\
F_i + mg = 0, \\
T_i = 0,
\end{array} \right.
\end{equation}
where  $m$  denotes the mass of the identical particles adjusted for buoyancy,  $g$  the gravitational acceleration,  $F_i$  (resp.  $T_i$ ) the drag force (resp. the torque) applied by the fluid on the  $i^{\text{th}}$  particle  $B_i$  defined as
\begin{eqnarray*}
F_i &:=& \int_{\partial B_i} \sigma(u^N, p^N) n, \\
T_i &:=& \int_{\partial B_i} (x - x_i) \times [\sigma(u^N, p^N) n],
\end{eqnarray*}
with  $n$  the unit outer normal to  $\partial B_i$  and  $\sigma(u^N, p^N) = 2 D(u^N) - p^N \mathbb{I}$ , the stress tensor where  $2D(u^N) = \nabla u^N + \nabla u^N^\top$ .

```

The XML snippet of the Stokes equation (via application of LaTeXML)

```
</Math> immersed in a viscous fluid satisfying the following Stokes equation:  
<!-- ***** mecherbet.sedimentation.tex Line 50 **** --&gt;&lt;/p&gt;<br/><equation frefnum="(1)" labels="LABEL: eq_stokes" refnum="1" xml:id="S1.E1">  
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```

A MathML (PM) snippet of the model (via LaTeXML)

So far some ideas about the use of the publications-based approach for mathematical information.

Thanks for your attention!

Contact

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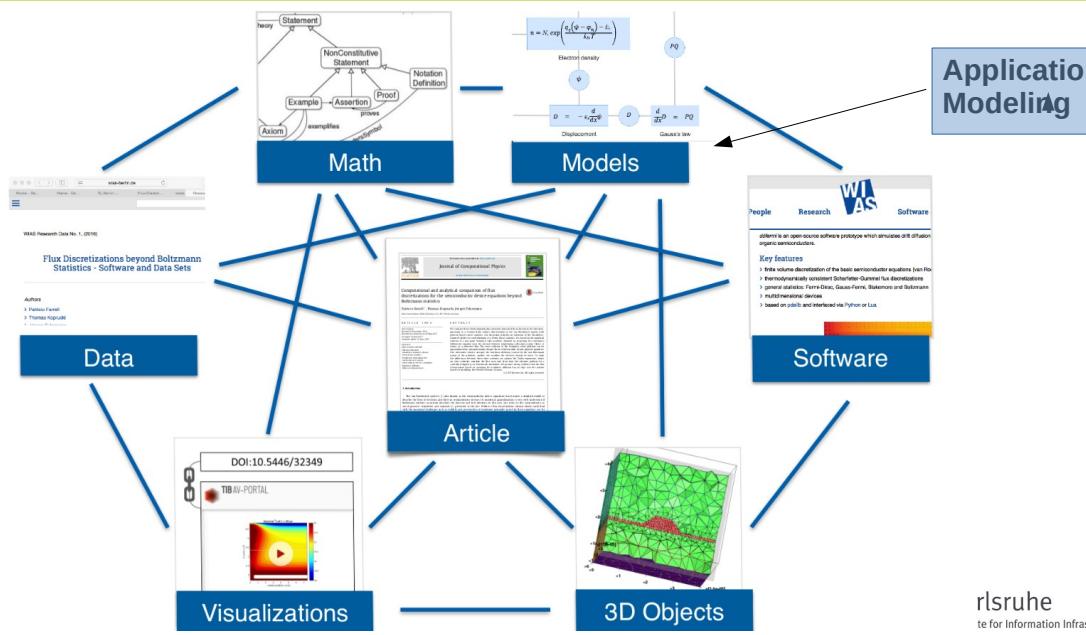
RISC, Hagenberg
2018-08-13

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OUTLOOK



The central role of mathematical models

A slide of Thomas



The goal and the idea

Building up a useful service for mathematical models:

- Thomas/Michael: Models play a central role for mathematical research
- How can we build a useful service for mathematical models?

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For humans:

In Title: Modeling

in Abstract: modeling: 'By coupling the van Roosbroeck equation with a quantum master equation in Lindblad form, ...'

in Introduction: → Model Equations in Sec. II

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$$\partial_t n - \frac{1}{q} \nabla \cdot \mathbf{j}_n = -R - S_n(\rho; n, p, \psi), \quad (2)$$

$$\partial_t p + \frac{1}{q} \nabla \cdot \mathbf{j}_p = -R - S_p(\rho; n, p, \psi), \quad (3)$$

$$\frac{d}{dt} \rho = \mathcal{L}(\rho; n, p, \psi) = -\frac{i}{\hbar} [H, \rho] + \mathcal{D}(\rho; n, p, \psi) \quad (4)$$

on the domain $\Omega \subset \mathbb{R}^3$. The system (1)-(4) is subject to initial conditions and boundary conditions modeling electrical contacts and other interfaces [32]. See Appendix A

→ Model Consistency III
→ Application

What is the model in the paper?

in textual form:

'hybrid quantum-classical model that self-consistently couples semi-classical transport theory to a kinetic equation for the quantum mechanical density matrix.'

as mathematical expressions (equations):

$$-\nabla \cdot \varepsilon \nabla \psi = q(p - n + C + Q(\rho)), \quad (1)$$

$$\partial_t n - \frac{1}{q} \nabla \cdot \mathbf{j}_n = -R - S_n(\rho; n, p, \psi), \quad (2)$$

$$\partial_t p + \frac{1}{q} \nabla \cdot \mathbf{j}_p = -R - S_p(\rho; n, p, \psi), \quad (3)$$

$$\frac{d}{dt} \rho = \mathcal{L}(\rho; n, p, \psi) = -\frac{i}{\hbar} [H, \rho] + \mathcal{D}(\rho; n, p, \psi) \quad (4)$$

on the domain $\Omega \subset \mathbb{R}^3$. The system (1)–(4) is subject to initial conditions and boundary conditions modeling electrical contacts and other interfaces [32]. See Appendix

But

- the model is incomplete: (1)-(4) are the partial differential equations. They must be completed by initial- and boundary equations
→ appendix (This is trivial for the mathematicians.)
- the model is specified (some hypotheses for the application case):
 - (1)-(4) are the basic equations
 - (1)-(3) van Roosbroeck (semi-classical transport model for electrons and holes)
 - (4) quantum master equation
- there are additional equations and principles which are presented in the subsection A, B, C and section III (evaluation of modeling: correctness accordance with the principles of thermodynamics).
- *Remark: This paper describes the modeling process (the model is the result of this paper), not the mathematical treatment of the model.*

A first summary

- The model is given by text and formulae.

For the mathematical treatment the formulae are the most important part. Often the textual environment gives some information about the meaning of the expression and the background of the model (origin / use cases) but can contain also structural information as in the example (van Roosbroeck, quantum master equation in Lindblad form, links to scientific theories, algorithms, software, ...)

- Both the textual information and the mathematical expressions which describe a model are relevant.
- Therefore we should try to extract both
 - the mathematical expressions describing the model
 - the corresponding terms and phrases for the mathematical expressions
- *Remark: Terms, phrases and mathematical expressions are ambiguous, but mathematical expressions, especially complex objects as equations, inequalities, structural diagrams contain precise information about their structure which allow to compare these objects and enhanced retrieval features.*

What can we do automatically?

➤ **The publication-based approach for mathematical models**

Up to now, models are part of publications. →Therefore we have to develop methods to extract the

- mathematical expressions describing the mathematical model and the corresponding terms and phrases.

Remarks:

➤ Fulltexts:

The most abstracts or reviews, the zbMATH data, don't contain precise model descriptions.

Typically, the mathematical expressions are not part of the abstract or reviews. Therefore, we need the fulltexts of the models.

➤ Formats:

Up to now, no powerful converter exists for transforming PDF formatted documents to TeX or MathML. At least, TeX encoded documents are needed. Therefore the arXiv e-prints are a first resource to develop methods for model analysis.

The publication-based approach

The publication-based approach covers three steps:

1) Identification of the model-relevant parts of the publication

- Model relevant sections or subsections
 - which can be identified by characteristic terms in the titles, especially 'model*' or 'problem*'
 - alternatively
 - the beginning of a document, e.g., the first 3,000 characters

A statistic

Journal	(Sub-)sections containg the terms `model' or `problem'
International Journal of Robust and Nonlinear Control, v. 10, n. 28	8 (9)
International Journal of Robust and Nonlinear Control v. 10, n. 29	6 (8)
Journal of System Science & Complexity v. 31, n. 3	7 (13)
Cybernetics and System Analysis v. 54, n. 2	8 (18)
International Journal of Control and Signal Processing v. 32, n. 6	7 (10)
Automation and Remote Control, v. 79, n. 5	6 (12)

Identification of model-relevant parts: results and open questions

by eliminating the non-relevant parts we get reduced (TeX-encoded) artifacts which contain only the model-relevant parts

- *Remark: It is not clear that the model-relevant parts contain only one model information. The reduced document can also contain previous models, similar models, specific models, generalized models, transformed models, etc.). In other words, it may contain a lot of additional information. How can we eliminate redundant / irrelevant information? (If yes, we could markup the model in the original file by a 'model tag')*

Our example: The section II contains ~ 100 mathematical expressions
9 / A:22 / B:29 / C:18 / fig.2:(15) text:10) (moreover, the mathematical expression from appendix A must be added).

The frequencies of some expressions is > 1.

Analysis of the model-reduced documents

2) Analysis of our artifacts:

- 1) extraction of all mathematical expressions (TeX or MathML encoded expressions) and the corresponding terms and phrases

→ creating a 'model-related' matrix A_{i_3} ($1 \leq i \leq n$, n – number of mathematical expression in the model-reduced document) for a document with the components :

a_{i_1} : mathematical expression

a_{i_2} : left-hand textual neighborhood (k terms)

a_{i_3} : right-hand textual neighborhood (k terms)

Example: C	doping profile	0
$Q(p)$	expectation value of the charge density	0
n	free electron density	0
p	free hole density	0
(1)-(3)	0	van Roosbroeck system

Analysis of the model-reduced documents: results and open questions

storing in a database ($A_{i_3}^k$ with k as the number of k -th document)

Remarks: As result we get a tensor which contains mathematical expressions plus their neighborhood. The mathematical expressions are listed in the sequence of their occurrence. This can make difficulties, e.g., parts of the model are presented at different positions in the document.

Can we identify the input variables of the model?

How can we organize it in a better way (sorting by length is not a real good idea)?

How can we identify the system structure of a model?

How can we find relevant textual information for a mathematical expression which is not in the left- or in the right-hand neighborhood of a mathematical expression?

What do we do with this information (e.g., storing this information in a special field of the tensor)?

Further processing: Transformation of the TeX-encoded mathematical expressions

3) It is difficult to compare TeX-encoded mathematical expressions

(the TeX codes for a PDF document differ; zbMATH experience: mathematical expressions with more than 6 characters occur in the database zbMATH only once)

better (more standardized): XML / MathML encoded mathematical expression
(tree structured documents)

MathML transformation of mathematical expressions via **LaTeXML**

→ tree-structured documents which allow to compare the structure of mathematical formulae

Remarks: LaTeXML transform the TeX code to XML. By postprocessing, the XML code can be transformed to MathML (Presentation Markup, Content Markup, or OpenMATH)

Which format should be used for storing, all or only MathML Content Markup?

(If the authors would write their documents in STeX, MathML or OpenMATH should be used).

Example (the PDE system 1 - 4)

```
\begin{align}
-\nabla \cdot \nabla \psi &= q(\rho - n + C + Q), \\
\partial_t n - \frac{1}{q} \nabla \cdot (\mathbf{j}_n) &= -R_S(n) \rho, \\
\partial_t p + \frac{1}{q} \nabla \cdot (\mathbf{j}_p) &= -R_S(p) \rho, \\
\frac{m d}{(m d t) \rho} = L(\rho, n, p, \psi) &= -\frac{i}{\hbar} (H \rho + D(\rho, n, p, \psi)). 
\end{align}
```

The Online Editor of LaTeXML

 ItxMojo: LaTeXML's Web Server

No obvious problems (Details)

About Upload & Convert Web Editor Help

```
1 \begin{align}
2   \nabla\cdot\mathbf{v}+\partial_t\psi-\nabla\cdot\nabla\psi &= -q\left(p-n+C+Q\right)\nabla\cdot\mathbf{v}, \quad \text{label{eq: Poisson equation}}
3   \partial_t\left(\nabla\cdot\mathbf{v}\right) &= -R_S(n)\nabla\cdot\mathbf{v}-R_S(p,\psi), \quad \text{label{eq: electric transport}}
4   \partial_t\left(\mathbf{v}\cdot\mathbf{J}\right)+\frac{1}{q}\nabla\cdot\mathbf{v} &= -R_S(p)\nabla\cdot\mathbf{v}-R_S(n,p,\psi), \quad \text{label{eq: hole transport}}
5   \frac{\partial}{\partial t}\left(\rho n\right)-\frac{1}{q}\nabla\cdot\mathbf{J}_n &= -R_S(n,p,\psi), \quad \text{label{eq: quantum master equation}}
6 \end{align}
```

On-the-Fly Preview

$$\begin{aligned} -\nabla \cdot \mathbf{v} \nabla \psi &= q(p - n + C + Q(\rho)), \\ \partial_t n - \frac{1}{q} \nabla \cdot \mathbf{J}_n &= -R - S_n(\rho; n, p, \psi), \\ \partial_t p + \frac{1}{q} \nabla \cdot \mathbf{J}_p &= -R - S_p(\rho; n, p, \psi), \\ \frac{d}{dt} \rho = \mathcal{L}(\rho; n, p, \psi) &= -\frac{i}{\hbar} [H, \rho] + \mathcal{D}(\rho; n, p, \psi) \end{aligned}$$


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```

ref5</cite>. The node equation read</p>
<math display="block">\text{equation refnum="1" label="LABELseq_Poisson_equation" refnum="S2_E1" fragid="S2_E1">
<math>\frac{\partial}{\partial t}\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{\text{center}}\left(r\right) \quad \text{(1)}
</math>
<math display="block">\text{fragid="S2_E1_a1">} \text{math alttext="displaystyle=\nabla\cdot\rho\nabla\psi+\rho\nabla\cdot\mathbf{E}-\rho\mathbf{E}\cdot\nabla\psi-\frac{q}{m}(\nabla\phi\cdot\nabla\psi)-\frac{q}{m}(\nabla\phi\cdot\nabla\phi)\delta_{center}(r)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(1)
<math display="block">\text{alttext="displaystyle=\rho\partial_t\psi+\nabla\cdot(\rho\nabla\psi)-\rho(\mathbf{E}\cdot\nabla\psi)-\frac{q}{m}(\nabla\phi\cdot\nabla\psi)-\frac{q}{m}(\nabla\phi\cdot\nabla\phi)\delta_{center}(r)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(2)
<math display="block">\text{fragid="S2_E1_a2">} \text{math alttext="displaystyle=\rho\partial_t\psi+\nabla\cdot(\rho\nabla\psi)-\rho(\mathbf{E}\cdot\nabla\psi)-\frac{q}{m}(\nabla\phi\cdot\nabla\psi)-\frac{q}{m}(\nabla\phi\cdot\nabla\phi)\delta_{center}(r)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(3)
<math display="block">\text{fragid="S2_E1_a3">} \text{math alttext="displaystyle=\rho\partial_t\psi+\nabla\cdot(\rho\nabla\psi)-\rho(\mathbf{E}\cdot\nabla\psi)-\frac{q}{m}(\nabla\phi\cdot\nabla\psi)-\frac{q}{m}(\nabla\phi\cdot\nabla\phi)\delta_{center}(r)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(4)
<math display="block">\text{fragid="S2_E2_a1">} \text{math alttext="displaystyle=\partial_t\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{center}\left(r\right)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(1)
<math display="block">\text{fragid="S2_E2_a2">} \text{math alttext="displaystyle=\partial_t\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{center}\left(r\right)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(2)
<math display="block">\text{fragid="S2_E2_a3">} \text{math alttext="displaystyle=\partial_t\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{center}\left(r\right)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(3)
<math display="block">\text{fragid="S2_E2_a4">} \text{math alttext="displaystyle=\partial_t\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{center}\left(r\right)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(4)
<math display="block">\text{fragid="S2_E3_a1">} \text{math alttext="displaystyle=\partial_t\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{center}\left(r\right)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(1)
<math display="block">\text{fragid="S2_E3_a2">} \text{math alttext="displaystyle=\partial_t\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{center}\left(r\right)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(2)
<math display="block">\text{fragid="S2_E3_a3">} \text{math alttext="displaystyle=\partial_t\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{center}\left(r\right)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(3)
<math display="block">\text{fragid="S2_E3_a4">} \text{math alttext="displaystyle=\partial_t\left(\rho\psi\right) + \nabla\cdot\left(\rho\nabla\psi\right) = \rho\left(\nabla\cdot\mathbf{E}\right) - \rho\left(\mathbf{E}\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\psi\right) - \frac{q}{m}\left(\nabla\phi\cdot\nabla\phi\right)\delta_{center}\left(r\right)" style="display:inline-block; width:100%; text-align:center; font-size:small; margin-bottom:10px;">(4)

```

XML ▾ Tab Width: 8 ▾ Line 142, Col 253 ▾ INS

Some remarks and questions

All mathematical expressions of our model description tensor could be transformed on this way to MathML PM or CM or OpenMATH. This allows to use graph-based models, e.g. for comparing models or retrieval.

➤ **The advantage of the approach:**

All steps of the publication-based approach can be done widely automatically.

But the method has also some disadvantages:

In principle our model tensors of publications should contain the model information, but it is possible that the information is too much. How can we remove model-irrelevant information?

Big tensors describing a model are not very impressive for the user. How can we compactify the model representations

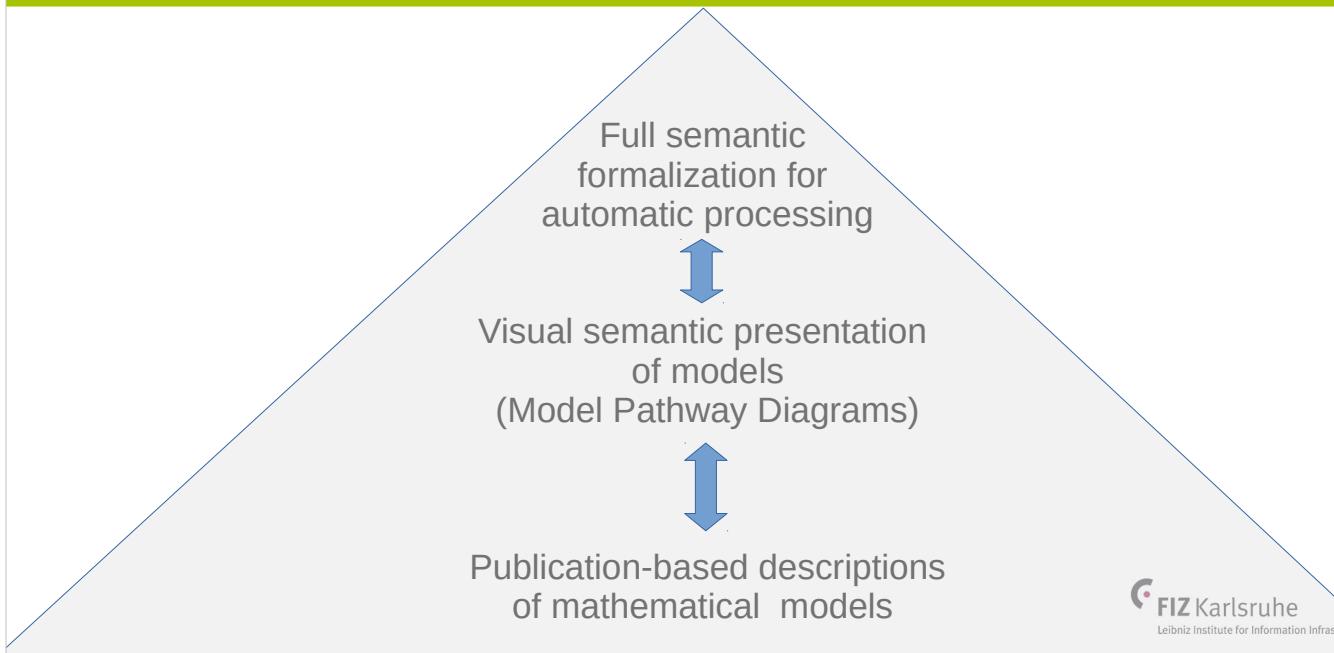
(A first idea:

A grouping of complex mathematical expressions with the involved notations should be possible. Often long mathematical expression are complex expressions (especially PDEs) containing special symbols which we could connect).

Further questions

- What is with retrieval (access for mathematicians and for non-mathematicians)?
- How can we detect similar models (ranking of the mathematical expressions of the models)?
- How can we make the service interactive (for improving the model, linking to further model information)?
- How can we make the modeling process understandable?

Our ambitioned goal: Building up a knowledge base for mathematical models



1. INTRODUCTION

In this paper, we consider a system of N spherical particles $(B_i)_{1 \leq i \leq N}$ with identical radii R immersed in a viscous fluid satisfying the following Stokes equation:

$$(1) \quad \begin{cases} -\Delta u^N + \nabla p^N = 0, & \text{on } \mathbb{R}^3 \setminus \bigcup_{i=1}^N \overline{B_i}, \\ \operatorname{div} u^N = 0, & \end{cases}$$

completed with the no-slip boundary conditions:

$$(2) \quad \begin{cases} u^N = V_i + \Omega_i \times (x - x_i), & \text{on } \partial B_i, \\ \lim_{|x| \rightarrow \infty} |u^N(x)| = 0, & \end{cases}$$

where $(V_i, \Omega_i) \in \mathbb{R}^3 \times \mathbb{R}^3$, $1 \leq i \leq N$ represent the linear and angular velocities,

$$B_i := B(x_i, R).$$

We describe the intertialess motion of the rigid spheres $(B_i)_{1 \leq i \leq N}$ by adding to the instantaneous Stokes equation the classical Newton dynamics for the particles $(x_i)_{1 \leq i \leq N}$:

$$(3) \quad \begin{cases} \dot{x}_i = V_i, \\ F_i + mg = 0, \\ T_i = 0, \end{cases}$$

where m denotes the mass of the identical particles adjusted for buoyancy, g the gravitational acceleration, F_i (resp. T_i) the drag force (resp. the torque) applied by the fluid

¹

Example 2:
The model
description
in the e-print
[arXiv:1806.07795](https://arxiv.org/abs/1806.07795)

2

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on the i^{th} particle B_i defined as

$$\begin{aligned} F_i &:= \int_{\partial B_i} \sigma(u^N, p^N) n, \\ T_i &= \int_{\partial B_i} (x - x_i) \times [\sigma(u^N, p^N) n], \end{aligned}$$

with n the unit outer normal to ∂B_i and $\sigma(u^N, p^N) = 2D(u^N) - p^N \mathbb{I}$, the stress tensor where $2D(u^N) = \nabla u^N + \nabla u^{N\top}$.

The publicly available TeX-code

```

\section{Introduction}
In this paper, we consider a system of  $N$  spherical particles  $\{B_i\}_{1 \leq i \leq N}$  with identical radii  $R$  immersed in a viscous fluid satisfying the following Stokes equation:
\begin{equation} \boxed{\begin{aligned} & \nabla \cdot u = 0, \\ & \Delta u - \nabla p = f, \\ & \nabla \cdot u = 0, \\ & u = 0 \text{ on } \partial \Omega, \end{aligned}} \quad \text{on } \mathbb{R}^3 \setminus \bigcup_{i=1}^N \overline{B_i}, \quad \forall t \in [0, T], \end{equation}
where  $u$  is the velocity field,  $p$  is the pressure,  $f$  is the body force, and  $\Omega$  is the domain. This equation is completed with the no-slip boundary conditions:
\begin{equation} \boxed{u = 0 \text{ on } \partial \Omega}, \quad \forall t \in [0, T]. \end{equation}
We describe the motion of the rigid spheres  $\{B_i\}_{1 \leq i \leq N}$  by adding to the previous Stokes equation the classical Newton dynamics for the particles  $\{x_i\}_{1 \leq i \leq N}$ :
\begin{equation} \boxed{\boxed{\begin{aligned} m \ddot{x}_i + \nabla \cdot \Omega_i \times x_i + \Omega_i \times (\nabla \times x_i) + \nabla p_i + \nabla \cdot f_i + \nabla \cdot g_i &= F_i, \\ \Omega_i \cdot \dot{x}_i &= 0, \end{aligned}}} \quad \forall i = 1, \dots, N, \end{equation}
where  $m$  denotes the mass of the identical particles adjusted for buoyancy,  $\nabla p_i$  the gravitational acceleration,  $F_i$  is the drag force (resp., the torque) applied by the fluid on the  $i$ -th particle  $B_i$  defined as
\begin{equation} \boxed{F_i = -\int_{\partial B_i} (\partial B_i) \cdot \nabla p_i \, d\sigma, \quad T_i = -\int_{\partial B_i} (\partial B_i) \cdot (\nabla \times x_i) \, d\sigma}, \end{equation}
with  $n$  the unit outer normal to  $\partial B_i$  and  $\nabla p_i \cdot n = 2 D(u) \cdot n + \nabla u \cdot n$ , where  $D(u) = \frac{1}{2} \nabla u \nabla u^T$ .

```

The XML snippet of the Stokes equation (via application of LaTeXML)

```

<Math> immersed in a viscous fluid satisfying the following Stokes equation:
<!-- %**** mecherbet sedimentation.tex Line 50 **** --></p>
<equation frefnum="(1)" label="LABEL: eq_stokes" refnum="1" xml:id="S1.E1">
  <Math mode="display" tex="(\left\{\begin{array}[]\right.\Delta u^N) + \nabla p^N = 0, \\ \operatorname{div}(u^N) = 0, \\ \overline{u^N} = 0, \\ \left.\begin{array}[](-\Delta u^N) + \nabla p^N = 0, \\ \operatorname{div}(u^N) = 0\end{array}\right. \quad \text{on } \mathcal{R}^3 = \Omega \cap B_1, \quad \text{with } u^N = 0 \text{ on } \partial\Omega \cap B_1." text="cases(@{Array[[- \Delta u^N + \nabla p^N, =, 0], [div(u^N, =, 0)]]} * [ on \mathcal{R}^3 = \Omega \cap B_1, ])" xml:id="S1.E1.1">
    <XMath>
      <XMap>
        <XMTok meaning="times" role="MULOP"></XMTok>
        <XMDual>
          <XMap>
            <XMTok meaning="cases"/>
            <XNRef idref="S1.E1.m1.3"/>
          </XMap>
        <XMWrap>
          <XMTok role="OPEN" stretchy="true"></XMTok>
          <XMArry role="ARRAY" vattach="middle" xml:id="S1.E1.m1.3">
            <XMRow>
              <XMCell align="right">
                <XMap>
                  <XMTok meaning="plus" role="ADDOP">&lt;&gt;</XMTok>
                  <XMap>
                    <XMTok meaning="minus" role="ADDOP">&lt;&gt;</XMTok>
                    <XMap>
                      <XMTok meaning="times" role="MULOP"></XMTok>
                      <XMTok name="Delta" role="UNKNOWN">&Delta;</XMTok>
                      <XMap>
                        <XMTok role="SUPERSCRIPTTOP" scriptpos="post8"/>
                        <XMTok font="italic" role="UNKNOWN">u</XMTok>
                        <XMTok font="italic" fontsize="70%" role="UNKNOWN">N</XMTok>
                      </XMap>
                    </XMap>
                  </XMap>
                </XMCell>
              </XMRow>
            </XMArry>
          </XMWrap>
        </XMDual>
      </XMap>
    </XMath>
  </equation>

```

A MathML (PM) snippet of the model (via LaTeXML)

So far some ideas about the use of the publications-based approach for mathematical information.

Thanks for your attention!

Contact

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