

Methods Training

Scholarship, Posters and Thesis

(English)

Dr. Karl N. Kirschner

Spring 2018

Day	Date	Session	Topic
1	13-02-2019	Morning (9:00 – 12:00)	Introduction
1	13-02-2019	Morning	Scholarship and research
1	13-02-2019	Morning	Taking notes
1	13-02-2019	Afternoon (13:00 – 15:30)	Posters
1	13-02-2019	Afternoon	Intro to Linux, desktop, command line
1	13-02-2019	Afternoon (15:30 – 18:00)	Personal working time (poster)
2	14-02-2019	Morning	Citations
2	14-02-2019	Morning	Literature searching and bibtex files
2	14-02-2019	Morning	Reference management (Citavi and Jabref)
2	14-02-2019	Afternoon	Inkscape & (Python3 ?)
2	14-02-2019	Afternoon	Personal working time (poster)
3	15-02-2019	Morning	Research questions and hypotheses
3	15-02-2019	Morning	Writing your thesis and personal time line
3	15-02-2019	Morning	FAQ thesis, LATEX
3	15-02-2019	Afternoon	Personal working time (poster)
	17-02-2019	Night (21:00)	Final PDF uploaded to LEA
4	18-02-2019	Morning 9:00	Poster PDF must be delivered to printshop
4	18-02-2019	Morning (1 hr)	Git
4	18-02-2019	Morning 10:00	Library seminar
4	18-02-2019	Afternoon	Significant figures and rounding
4	18-02-2019	Afternoon	Personal working time
5	19-02-2019	Morning	Ethics
5	19-02-2019	Morning	Course evaluations
5	19-02-2019	Afternoon	Poster presentation
	??-??-2019	08:00-11:00	Poster Session at the Niehl training center

Questions or comments from last lecture(s)?

German and English Thesis Examples and Template:

https://gitlab.com/k.n.kirschner/H-BRS_Thesis_Template.git

FAQ About Thesis:

LEA → EMT-Studieninfos → Prüfungen → FAQ →
Häufige Fragen zu Prüfungsangelegenheiten →
Prüfungsinformationen für alle EMT-Studiengänge: →
Fragen zur Abschulssarbeit und zum Kolloquium

Bib-Cloud – <https://www.h-brs.de/en/bib/cloud-storage-keep-your-files-safe-bibcloud>

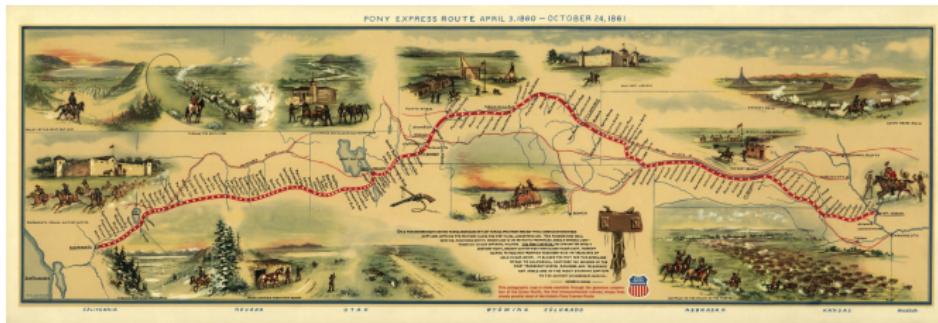
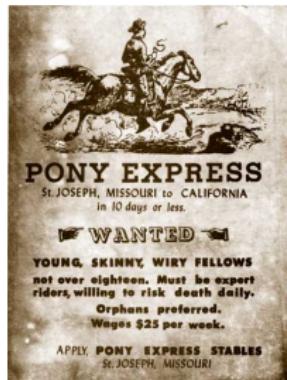
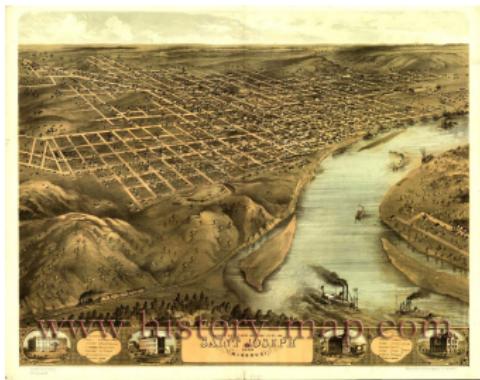
Personal Introduction

Germany to the US

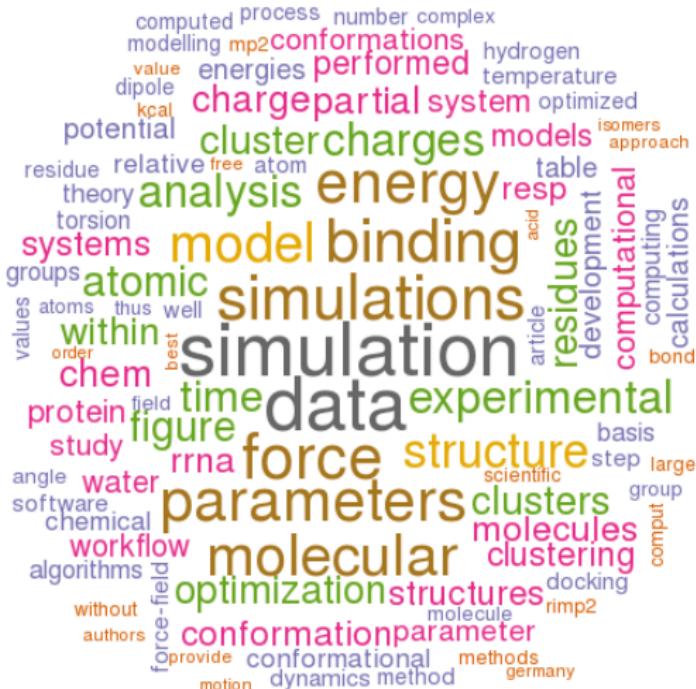


Immigration ~1840 ... and back again in 2007

Saint Joseph, Missouri



- Ph.D. in physical chemists (1999)
- Professor at Hamilton College (2004-2008)
- Senior researcher at Fraunhofer SCAI (2008-2013)
- H-BRS researcher, dozent, Int. Chair (2014-now)
- > 50 publications



Mentoring students in research



Hamilton College 2007

Since being in
Germany

- FhG SCAI
- H-BRS
- Uni Bonn
- H-BRS
- 4 PhD
- 6 master
- 6 bachelor

Course Introduction

Background

- Method Training - bachelor thesis
 - Possibly your first introduction to being scholarly
 - Involves a “simple” project → 4 month time period

- What is this course about (i.e. my goals)?
 - To inform you of some of the department's and university's rules for bachelor thesis (and personal time management)
 - To introduce some new ideas - increase your knowledge concerning research and scholarship.
 - To provide you some solutions for solving problems that you might come across during your research.
 - To make you better scholars!

Your thesis is the end-product of your bachelor's education.

Thesis

- Research
 - Literature search and reference management (e.g. Citavi, Jabref)
 - Software and programming (e.g. Matlab)
- Dissemination (i.e. writing for conveying information)
 - Thesis sections (e.g. Introduction, Methodology)
 - Software (e.g. calc, excel, illustrator, inkscape, Python3, L^AT_EX)
 - Data organization (e.g. csv files)
 - Tables
 - Figures
 - Citations

Poster - a condensed version of what you will need to do for your thesis

Some philosophy to start the course.

Who are you?

A difficult question to answer.

A person “is a **thinking** intelligent **being**, that has **reason** and **reflection**, and can consider itself as itself, the same thinking thing, in different times and places...”

– John Locke, Essay concerning Human Understanding

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Fundamentally, you are ...

- ... a collection of **thoughts** and beliefs
- ... a collection of emotions
- ... a collection of experiences - **acquired** (i.e. **learned**)
- ... and some things that you were born with (i.e. innate)

Thoughts and acquired experiences

Who do you want to become?

You can control the direction that you take to become that future self.

- 1 Create opportunities for you to acquire new experiences
(door opening opportunities)
 - Education
 - Traveling
 - Socializing
- 2 Cognitively decide what type of person/personality you want to be
(introspective)
 - Education
 - Reading
 - Reflections and thinking

Point 2 helps with point 1

And what of this course?

This is an opportunity for you to

- Learn new ideas, methods and approaches on
 - How to represent yourself to others (communication)
 - Become more focused with short- and long-term goals

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- Consider how you organize your thoughts and those of others (original ideas versus those of others) - we are all standing on the shoulders of giants.

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- Learn new ideas, methods and approaches on
 - How to represent yourself to others (communication)
 - Become more focused with short- and long-term goals
- Consider how you organize your thoughts and those of others (original ideas versus those of others) - we are all standing on the shoulders of giants.
- Purposely direct your thoughts/energy towards who you want to become.

Examples:

- conceptually precise, conceptually broad
- good with generating data, good with data analysis
- good with visual communication
- good with written communication
- good with oral communication
- reliable, honest
- reductionist versus holism

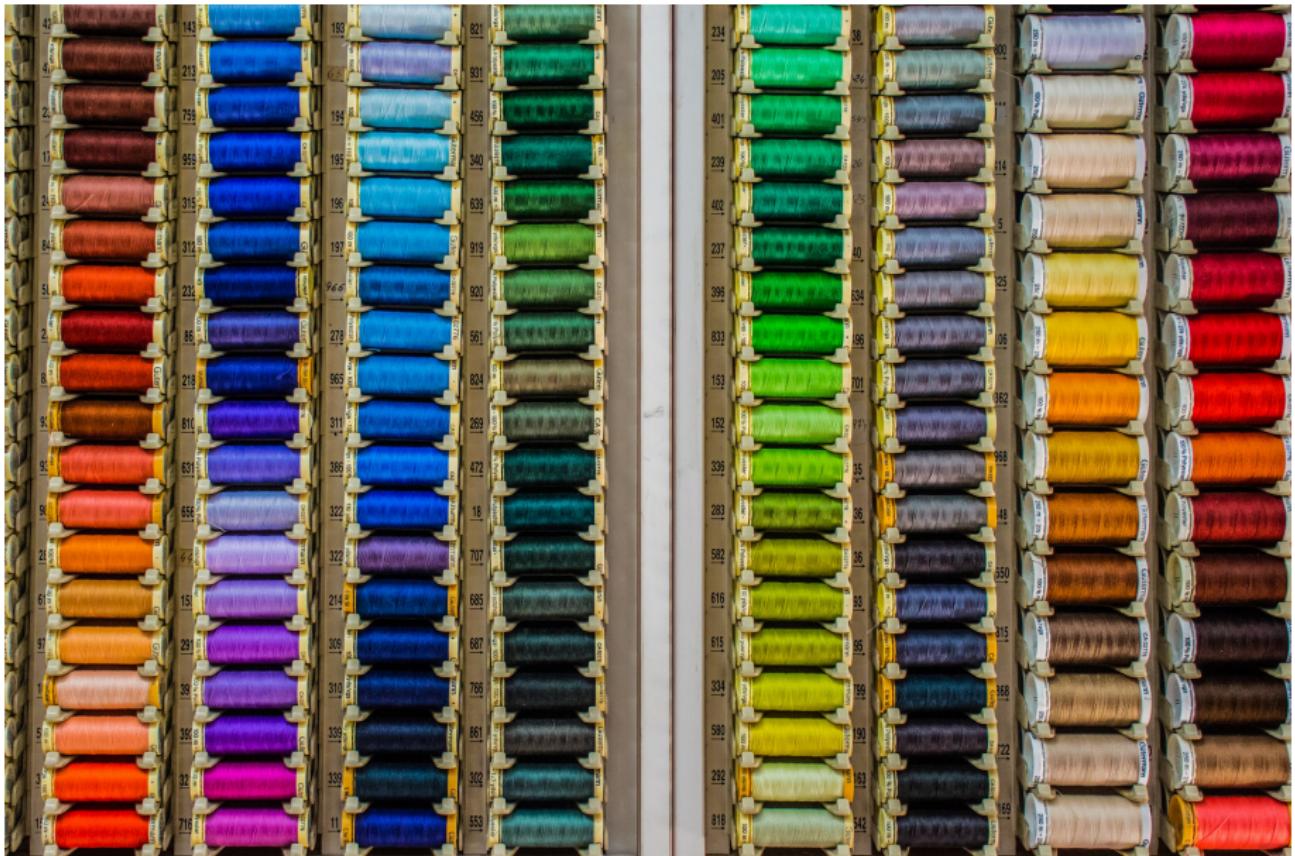


Photo by Héctor J. Rivas on Unsplash

Scholarship

True or Fake

- It is not what you eat, but how much exercise that determines weight.
 - Prof. Steven Blair, University of South Carolina
 - Prof. James O. Hill, University of Colorado
 - Gregory A. Hand, West Virginia School of Public Health
 - Principle scientists of Global Energy Balance Network company

- https://youtu.be/9xBV_Enlh1A

- A scientific study showed that young fish prefer to eat plastic microbeads instead of regular food.
 - Environmental Fish Protection Group, 2016 study

- Hot water cools faster (i.e.sooner) than cool water.
 - Lasanta, A.; Vega Reyes, F.; Prados, A. & Santos, A. When the Hotter Cools More Quickly: Mpemba Effect in Granular Fluids, Phys. Rev. Lett., 2017, 119, 148001.

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Is this done in a scholarly manner?

Table 1: Theory versus experiment from literature [1-4].

	Method 1	Error	Method 2	Error	Experiment	Year
Observable 1	3	2.9	2.9	2.9	2.9	2010
Observable 2	6.1	6.4	6.4	6.1	6.6	2010
Observable 3	3.9	3.6	3.9	3	3.7	2010
Observable 1	0.5	0.9	0.6	8.5	0.6	2015
Observable 2	4	0.5	0.8	0.2	5.2	2015
Observable 3	4.7	1.1	3.9	0.8	4.3	2015

Can you make this table better? If so, how?

Is this done in a scholarly manner?

Table 1: Theory versus experiment from literature [1-4].

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Observable 3	3.9	3.6	3.9	3.0	3.7	2010
Observable 1	0.5	0.9	0.6	8.5	0.6	2015
Observable 2	4.0	0.5	0.8	0.2	5.2	2015
Observable 3	4.7	1.1	3.9	0.8	4.3	2015

Is this done in a scholarly manner?

Table 1: The simulated value (error), in kg/m³, of the three observables using two methodologies (see Methods section) versus experimental values.

Observable	Method 1	Method 2	Experiment
Year: 2010			
1	3.0 (2.9)	2.9 (2.9)	2.9 ^a
2	6.1 (6.4)	6.4 (6.1)	6.6 ^b
3	3.9 (3.6)	3.9 (3.0)	3.7 ^c
Year: 2015			
1	0.5 (9.0)	0.6 (8.5)	0.6 ^d
2	4.0 (0.5)	0.8 (0.2)	5.2 ^d
3	4.7 (1.1)	3.9 (0.8)	4.3 ^d

^a Reference [1].

^b Reference [2].

^c Reference [3].

^d Reference [4].



Photo by Daniel Chekalov on Unsplash

Example 1

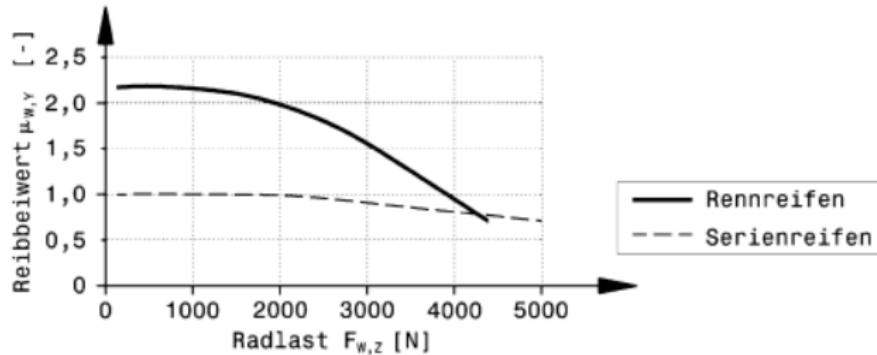


Abbildung 10: Reibwert in Querrichtung über Radlast - Mit zunehmender Radlast nimmt der Reibwert der Reifen ab. Der degressive Verlauf des Reibwertes von Reifenmischungen ist typisch.¹⁷

From an H-BRS Bachelor Thesis

Example 2

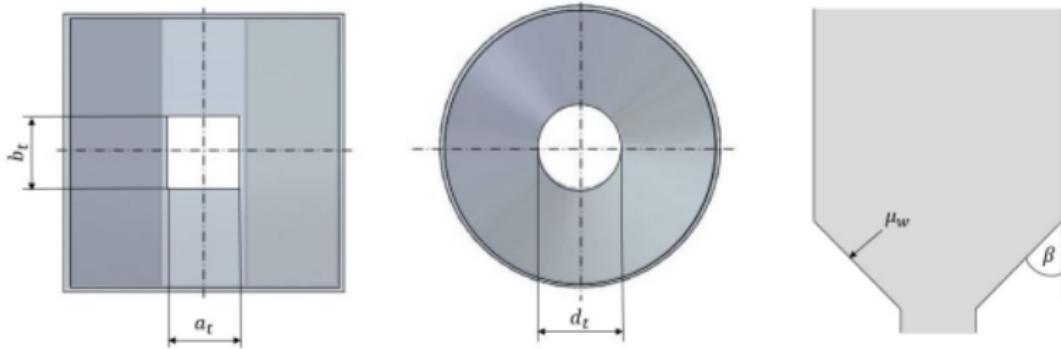


Abbildung 2.3: Silokenngrößen die einen Einfluss auf das Fließverhalten eines granularen Materials ausüben. Die Größe der Trichterauslauföffnung wird hier mit a_t und b_t oder dem Durchmesser d_t bezeichnet. Die Silowandreibung wird mit μ_w beschrieben und β beschreibt den Trichterwinkel.

From an H-BRS Bachelor Thesis

Example 2

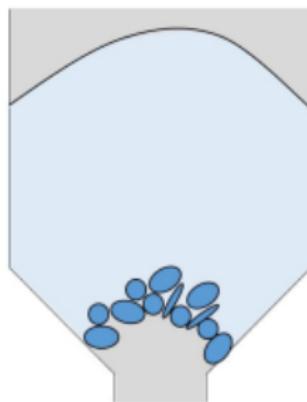


Abbildung 2.4: Brückenbildung in einem Silo. Die Partikel ordnen sich über der Trichterauslauföffnung an und verschließen das Silo.

From an H-BRS Bachelor Thesis

Example 2

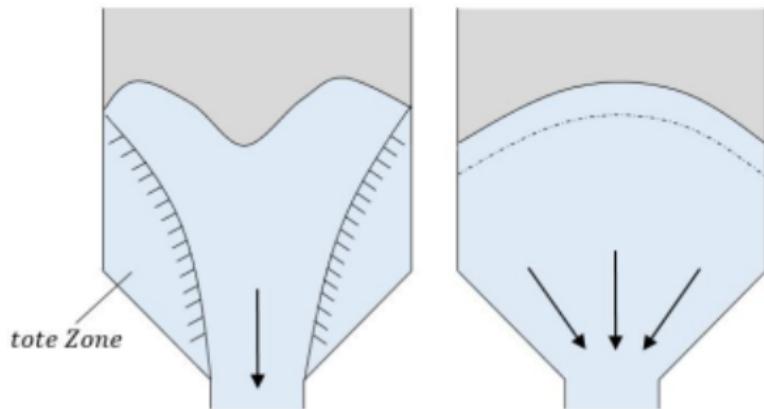


Abbildung 2.5: Darstellung eines Kernflusssilos (links) und Massenflusssilos (rechts). Bei einem Kernflusssilo bilden sich tote Zonen, in denen kein Materialfluss vorhanden ist. In einem Massenflusssilo ist der gesamte Inhalt in Bewegung.

From an H-BRS Bachelor Thesis

Example 3

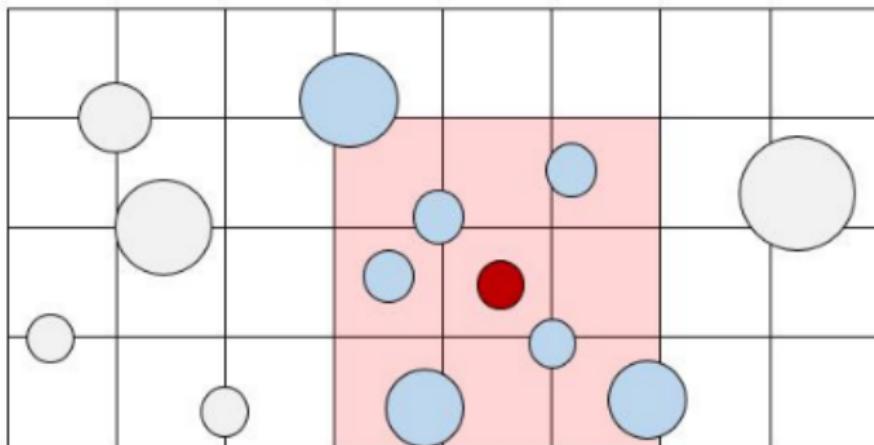


Abbildung 3.3: Zellenbasierte Methode zur Kontaktdetektion im zweidimensionalen Raum. Das Simulationsfeld wird in Achsenrichtung in ein Raster aus quadratischen Zellen (im dreidimensionalen Raum: kubischen Zellen) zerteilt. Die Partikel, die sich in der Zelle des zu beobachtenden Partikel (rot) und in deren direkten Nachbarzellen befinden, werden als mögliche Kontakte erkannt. Die restlichen Partikel werden ausgeschlossen.

Example 4

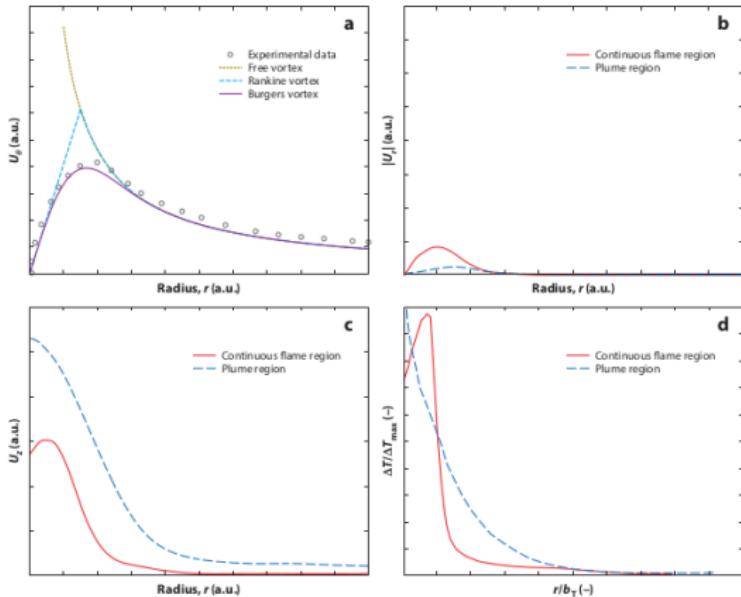


Figure 6

Velocity profiles predicted and measured for the inner and outer structure of an on-source, stationary fire whirl. (a) Azimuthal velocity U_ϕ as a function of radius r , including theoretical predictions and experimental data made by Hartl (2016) and Hartl & Smits (2016). (b) Radial velocities $|U_r|$ within the continuous flame and plume regions. (c) Axial velocities U_z measured within the continuous flame and plume regions by Hartl (2016). (d) Normalized excess temperature $\Delta T / \Delta T_{\max}$ measured against normalized radial distance r/b_T , with b_T measured within the continuous flame and plume regions by Lei et al. (2015b).

Tohidi, A.; Gollner, M. J. & Xiao, H., Fire Whirls, Annual Review of Fluid Mechanics, 2018, 50,

Example 6

Table 1: Selected internal coordinate values for methanol trans conformation.

Method	r_{CO}	r_{OH}	ϕ_{COH}	δ_{HCOH}
Minimum: t				
Exp. ^a	1.427	0.956	108.52	
Exp. ^b	1.427	0.953	108.24	
Exp. ^c	1.428	0.960	109	
Average	1.427	0.956	109	
MP2/aV5Z	1.419	0.958	108.22	61.4
CCSD(T)/DPZ ^d	1.429	0.964	107.6	61.5
CCSD(T)/VTZ ^e	1.421	0.959		
CCSD(T)/VTZ ^f	1.421 (1,418)	0.960 (0.958)	107.42 (107.51)	120
CCSD(T)/aVTZ ^e	1.425	0.961		
CCSD(T)/VQZ ^f	1.419	0.958	107.98	60
CCSD(T)/wCVQZ ^f	(1.416)	(0.957)	(108.08)	

a. Ref. [1]

b. Ref. [2]

c. Ref. [3]

d. Ref. [5] - note that the COH angle appears to be mislabeled in Table XII as COH₃.

e. Ref. [6] - note that the aVTZ basis sets was modified by removing the highest spin functions.

f. Refs. [7, 8] - the values in parenthesis are from all-electron correlated calculations.

- Descriptive title
- Consistent formatting.
- Good citations and concise notes to guide the reader in their understanding
- Significant figures in the average calculations

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...				
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...				

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...

d. Ref. [5] - note that the COH angle appears to be mislabelled in Table XII as COH₃.

Example

Fully relaxed density-fitted (DF) [15, 16] HF/6-31G(d) and Møller–Plesset second-order perturbation theory (MP2) [17] optimizations were performed on all minima and first-order saddle points until a maximum force of 1.5E-5, a root-mean-squared (RMS) force of 1.0E-5, a maximum displacement of 6.0E-5 and an RMS displacement of 4.0E-5 (i.e. a tight convergence) were achieved. The DF-MP2 optimization employed 6-31G(d), cc-pVTZ (VTZ), aug-cc-pVTZ (aVTZ), cc-pVQZ (VQZ), aug-cc-pVQZ (aVQZ) and aug-cc-pV5Z (aV5Z) basis sets [18-21].

Example

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- Clear and concise writing
- Well referenced
- References are in consecutive order
- Clarification and use of abbreviations.

Scholarship

Summarize together

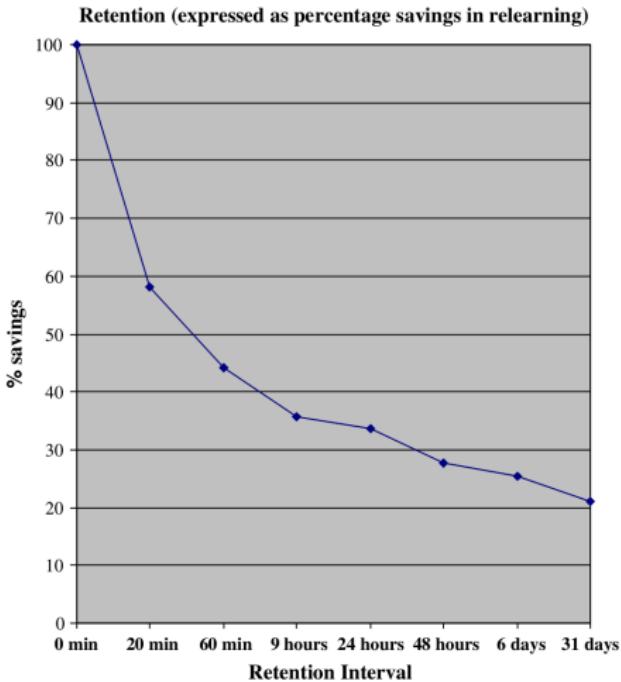
Taking Notes



Photo by Rob Wingate on Unsplash

The forgetting curve

Fig. 1 Example of an Ebbinghaus curve. Retention expressed as percentage savings while relearning the materials after the RI (Ebbinghaus learned until he achieved 100% correct trials). Based on Ebbinghaus (1966, p. 103)



E. J. F. M. Custers. Long-term retention of basic science knowledge: a review study.
Advances in Health Sciences Education, 15(1):109–128, Mar 2010

Why Take Notes?

- Keeps you alert
- Engages your mind
- Organizes information
- Creates a source for information and review
- **Helps you learn!**
 - comprehension
 - retention
 - one of the major ways that people learn
 - repetition when rewritten

“Note-taking ... can be used to predict ... a student's membership in either a higher achievement or lower achievement academic track”

B. J. Zimmerman and M. Martinez-Pons. [Construct validation of a strategy model of student self-regulated learning.](#)

Journal of educational psychology, 80(3):284, 1988

Basic Note Taking

- Make an outline of the topic being discussed
- Create a mind map
- Write out bullet points
- Highlight most important text (studying)
- Summarize in pictures
- Use abbreviations
 - & : and
 - # : number
 - ? : question
 - ! : important
 - ** : remember this
- Write clearly
- Ask questions

[http://www.millersville.edu/gened/files/PDFs%20Faculty%20Handbook/
11_Effective%20Note%20Taking%20Strategies.pdf](http://www.millersville.edu/gened/files/PDFs%20Faculty%20Handbook/11_Effective%20Note%20Taking%20Strategies.pdf)

What is important for your notes?

- Accuracy
 - Completeness
 - Organization (mirrors your understanding of the content)
 - Post-class processing and reviewing
-

E. J. F. M. Custers. Long-term retention of basic science knowledge: a review study.
Advances in Health Sciences Education, 15(1):109–128, Mar 2010

The Cornell System

Topic/Course	Source	Date
Cues Key Ideas & Questions Key Words Vocabulary Important Stuff	<h1>NOTES</h1> <p>Key words and ideas</p> <p>Definitions</p> <p>Important dates people places</p> <p>Brainstorming</p> <p>Diagrams and Pictures</p> <p>Formulas</p>	<i>Do after the notes have been taken</i>

<http://www.barstow.k12.ca.us/BHS/Class/271-AVID-Mrs-Barela/>

Assignments/4937-Math-Cornell-Note-Samples.html

<p><u>Close Notes</u> If there was no class lecture this week, write a paragraph about what you learned and/or questions about what you didn't understand.</p> <p><u>Topic:</u> Distance formula</p> <p><u>Questions/Main Ideas:</u></p> <p>What is the distance formula?</p>	<p>Name: <u>Student A</u></p> <p>Class: <u>Algebra</u></p> <p>Period: <u>6</u></p> <p>Date: <u>4/11</u></p> <p><u>Notes:</u></p> <p>The distance formula calculates distance based on rate and time.</p> <p>$D = r \cdot t$</p> <p>Example 1: How far will a train travel at 85 mph for 4 hours?</p> <p>$D = ?$ $r = 85 \text{ mph}$ $t = 4 \text{ hours}$</p> <p>$D = 85(4)$ $D = 340 \text{ miles}$</p> <p>Example 2: How far will a truck travel at 65 mph for 3.5 hrs?</p> <p>$D = ?$ $r = 65 \text{ mph}$ $t = 3.5 \text{ hrs.}$</p> <p>$D = 65(3.5)$ $D = 227.5 \text{ miles}$</p> <p>Summary: The distance formula measures distance based on rate and time. Distance = rate times time. This is often used with word problems.</p>
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English, Commas, Nov.1

Key Ideas

Series of adjectives

When should you use a comma between adjectives?

Commas with direct address

Page 44 in Readers
Notebook exp.
comma splice rules.

Comma Rules

Rule 1. Separate a series of three or more.

* My \$10,000,000 estate is to be split among my husband, dog, neighbor, and favorite son.

Rule 2. Use a comma to separate two adjectives when the word "and" can be put between them.

* He is a strong, healthy kid.

* We stayed at an expensive summer resort.

You would NOT say expensive and summer resort, so no comma.

Rule 3. Use commas before or surrounding the name or title of a person directly addressed.

* Will you, Aisha, hand this to Lily?

* Yes, Mrs. Roell, I will.

Comma Rules, ct'd. next page

Summary

Commas:

* lilacs, magnolias, roses, and daisies

* lovely, perfect day bc lovely & perfect day works

* Yo, Adrian, c'mere.

Visual/sketch note taking

Holly Clark - Meet Generation Z
Singapore November 11, 2017

My "poor" grampa

Me: who's calling? Had to get up to change channel! Generation Z are tech-dependent, not necessarily tech savvy.

Egs: Give away passwords

Short attention span (8 secs)

Highly connected

Social entrepreneurs

Kidz cation

WOAH! What will life be like in 14 years?

GROWTH HACK EDUCATION!

1 New literacies

- need to be transliterate
- How to develop Generation Z mindset?
- Maybe we will look back at our brutal treatment of animals
- 3D printing meat
- Sofia robot solving problems
- 13 years old on ESPN using an algorithm
- "The Connor Curve"
- Encouraged creativity
- Students now successful rappers "That's what dreams are made of!"
- Live outside your comfort zone
- Now at USC! HOORAY!
- Our kindies won't need to learn how to drive
- AI will replace 50% of jobs

2 Open & Transparent

@ Beverly Pham, rejected from U.S.C. → Made viral "Frozen" video

23 & me

Methods Training (English)

<https://www.flickr.com/photos/sylviaduckworth/with/24567013338/>



Photo by Francesco Cutolo on Unsplash

Posters



C. Woolston. Conference presentations: Lead the poster parade.

536:115–117, 2016

Posters

A poster's goal is to

- transfer knowledge
- obtain feedback
- network (if you go to a conference)

Posters are a hybrid form of communication

- Speech/Talk - presenter determine the focus
- Thesis/Paper - writer determine the focus
- Poster - the writer and viewer determines the focus
- Interview - the interviewer determines the focus

D. Ilic and N. Rowe. [What is the evidence that poster presentations are effective in promoting knowledge transfer? a state of the art review.](#)

Health Information & Libraries Journal, 30(1):4–12, 2013

A poster must ...

- ... communicate findings quickly
- ... grab attention
- ... be read from a distance (font size)
- ... have easy to follow text blocks
- ... incorporate graphics

Basic starting point

- Check the required format if any.
- Check the required size (A0, A1 etc.).
- Does it need to be landscape vs portrait?
- What is your time frame?
- Final poster format should be PDF (safest).

Focus on 1-3 important key points.

General guides: A poster's total words: 500–800

- Title
- Author and Affiliation
- Introduction - approx. 150 words
- Methodology - approx. 150 words
- Results - approx. 150–200 words
- Conclusion - approx. 150 words
- References - up to 5
- Acknowledgements - 40 words
- Contact information

K. D. Goldman and K. J. Schmalz. Poster session fundamentals: Becoming a proficient "poster child" for health education.

Health Promotion Practice, 11(4):445–449, 2010.

PMID: 20689050

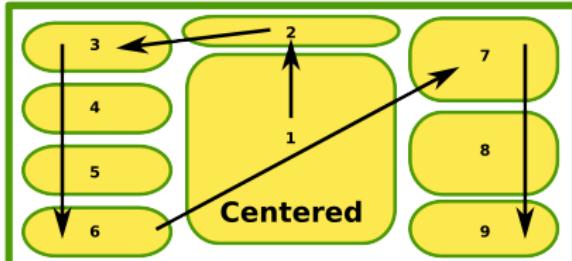
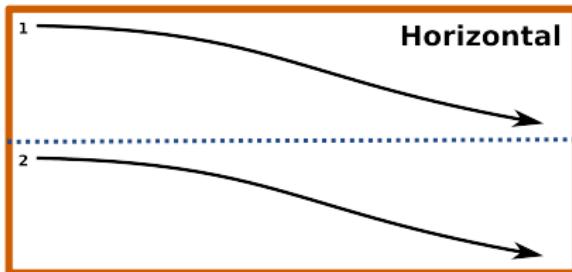
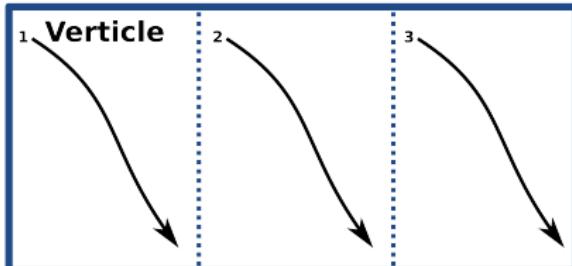
A0 and A1 poster font size

- Title: 85 pt
- Authors: 56 pt
- Subheadings: 36 pt
- Body: 24 pt
- Captions: 18 pt (never go below this)

Poster images

- At least 150 dpi
- No more than 300 dpi
- Format: **svg**, **png** and **jpg**

Designs



Tips

- Clean and simple light colored background
- Use a single font (i.e. Sans-Serif)

Sans-Serif: Arial, Helvetica, Geneva

AaBbCDEFGgHI

Serif: Times New Roman, Georgia, Garamond

AaBbCDEFGgHI

Monospace (e.g. code) : Courier

AaBbCDEFGgHI

AaBbCc

Sans-Serif

AaBbCc

Serif

(For those who go to a conference:)

- Post a version in the hallway weeks in advance – ask for feedback (use StickyNotes)
- Print on A4 for handing out at the conference session

Software for creation

- MS's PowerPoint, Libreoffice's Impress Presentation (easiest)
- Illustrator, Inkscape (a higher learning curve, but more flexible)

7 Simple Rules for a Good Poster Presentation

- 1 Sell your work in 10 seconds - you versus many other posters (e.g. 100 at a professional conference)
- 2 The title is important - make it inviting - short, sharp and compelling
- 3 Good writing also applies to posters (i.e. concise)

7 Simple Rules for a Good Poster Presentation

- 4 Layout and format are critical - guide the reader's eyes
- 5 Content is important, but keep concise - use graphics and charts
 - graphics - clear portrayal of the complex
 - charts - bold trend lines
- 6 Poster should have your personality
 - a way to draw in like-minded people (collaborations)
 - a photo of you on the poster (recognition outside of poster event)
- 7 Include an E-mail and URL (LinkedIn, Xing, ResearchGate, etc.)

T. C. Erren and P. E. Bourne. [Ten simple rules for a good poster presentation.](#)

PLOS Computational Biology, 3(5):1–2, 05 2007

Advanced poster ideas

- Add a physical model - catches the eye
- Add a QR code - enables more sophisticated things (e.g. movies, interaction)



C. Woolston. Conference presentations: Lead the poster parade.
536:115–117, 2016

Color schemes



Photo by Cody Davis on Unsplash

Color schemes

Color schemes can make a poster excellent or it can break a poster

- Better Colors - <http://colorbrewer2.org>
- COTW - <http://www.colorsontheweb.com>
- Paletton - <http://paletton.com>
- Adobe Color - <https://color.adobe.com>

Bad example 1

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O⁶-Benzylguanine Inhibits Tamoxifen Resistant Breast Cancer Cell Growth and Resensitizes Breast Cancer Cells to Anti-Estrogen Therapy

Joshua Smith¹, George C Bobustic¹, Rafael Madero-Vishal¹, Jimmie Colom¹, Beth Isley¹, Jonathan Ticku¹, Kalkunte S. Srivengopal and Santhi Konduuri^{1*}

¹Cancer Research Institute of M.D. Anderson Cancer Center Orlando /Texas Tech University Health Sciences Center, Amarillo, TX

Abstract

Endocrine therapies using aromatase inhibitors are first line and every option for breast cancer. However, tumor resistance to tamoxifen remains a stumbling block for successful therapy. Based on our recent study on the treatment of the ER⁺ resistant breast cancer cell line T47D with the anti-tumor agent O⁶-benzylguanine (O⁶-BG), we determined whether O⁶-BG inhibits ER⁺ mediated tumor cells. Specifically, we determined whether administration of O⁶-BG inhibits ER⁺ dependent gene expression and whether O⁶-BG enhances breast cancer cells to tamoxifen using tamoxifen resistant cells.

MD Anderson has been the first to demonstrate that tamoxifen does not inhibit ER⁺ breast cancer cells. The ER⁺ tumor cells significantly higher express the tamoxifen resistant MCF-7 compared to the parent cells. Likewise, the ER⁺ expression using a specific antibody was significantly lower in tamoxifen treated and parent cells levels by 1.5 fold. We also observed an increase in tamoxifen treated ER⁺ and pS2 levels in the control cells as compared to O⁶-BG treated cells. These observations were supported by increased MCF-7 expression. Other experiments showed that ER⁺ cells are ER⁺ in combination with tamoxifen and fluorescence microscopy indicated that ER⁺ cells have tamoxifen resistance. All these treatments increased the pS2/ER⁺ and pS2 expression significantly. ER⁺ inhibited tamoxifen resistance in T47D cells and decreased tamoxifen resistance in T47D cells. The T47D cells showed a decrease in tamoxifen induced estrogen receptor changes (TAM-ER). These combinations increased the endogenous C-erbb and pS2 expression, indicating that O⁶-BG inhibits ER⁺ dependent gene expression. ER⁺ cells exhibited the expression of MCF-7, ER⁺, ER⁺ and tamoxifen resistant genes. This study demonstrates that ER⁺ cells exhibit the expression of MCF-7, ER⁺, ER⁺ and tamoxifen resistant genes. Our results provide an alternate approach for endocrine resistant cells.

Introduction

Recent advances in breast cancer research have identified key pathways involved in the repair of DNA damage induced by chemosensitive agents. The ability of cells to repair or regenerate DNA damage and tolerate DNA repair is an important mechanism used by tumor cells to escape from therapeutic agents. The double strand break repair pathway and nucleotide excising repair attack the double-strand break repair mechanism and highly cytotoxic interstrand DNA crosslinks are produced. ER⁺ is a major pathway that is involved in cell proliferation and is responsible for protecting both tumor and normal cells from cytotoxic agents. MCF-7 is estrogen responsive and is considered to be a model system for breast cancer. Interestingly, it has been shown that tamoxifen modulates proliferation of MCF-7 cells and is responsible for protecting both tumor and normal cells from cytotoxic agents. MCF-7 is estrogen responsive and is considered to be a model system for breast cancer. Interestingly, it has been shown that tamoxifen modulates proliferation of MCF-7 cells and is responsible for protecting both tumor and normal cells from cytotoxic agents. MCF-7 is estrogen responsive and is considered to be a model system for breast cancer. Interestingly, it has been shown that tamoxifen modulates proliferation of MCF-7 cells and is responsible for protecting both tumor and normal cells from cytotoxic agents. MCF-7 is estrogen responsive and is considered to be a model system for breast cancer. Interestingly, it has been shown that tamoxifen modulates proliferation of MCF-7 cells and is responsible for protecting both tumor and normal cells from cytotoxic agents. MCF-7 is estrogen responsive and is considered to be a model system for breast cancer. Interestingly, it has been shown that tamoxifen modulates proliferation of MCF-7 cells and is responsible for protecting both tumor and normal cells from cytotoxic agents. MCF-7 is estrogen responsive and is considered to be a model system for breast cancer. Interestingly, it has been shown that tamoxifen modulates proliferation of MCF-7 cells and is responsible for protecting both tumor and normal cells from cytotoxic agents.

Interestingly, several observations suggest an inverse correlation between the levels of MCF-7 and tamoxifen responsive protein where wild-type pS2 represents responsiveness of MCF-7 expression. Unfortunately, ER⁺ function is often maintained after tamoxifen treatment, suggesting that tamoxifen resistant cells are still capable of responding to ER⁺ growth stimulatory responses. Whether, or where, at this is marked by upregulation of MCF-7 expression is to be determined. To determine whether tamoxifen resistant cells can respond to tamoxifen, we examined the response of tamoxifen resistant cells to tamoxifen treated normal breast cancer. The anti-tamoxifen treatments is the most commonly and treatment for patients with tamoxifen resistance. The tamoxifen resistance is a common problem in breast cancer. The tamoxifen resistance is associated with different types of mutations and altered ER⁺ function. ER⁺ is a modulator for MCF-7 which results in the reduction of tamoxifen sensitivity. Interestingly, ER⁺ cells are resistant to tamoxifen, suggesting that tamoxifen resistance is an ER⁺ mutation mechanism effectively reduces the MCF-7 treated in tamoxifen and the measured result of proliferation change. TAM-ER is tamoxifen resistance gene that is expressed in the cells treated with tamoxifen.

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Results

Prolonged Treatment of Tamoxifen Increases MCF-7 Expression: We developed a tamoxifen resistant MCF-7 cell line by using tamoxifen and it is called as "T47D cells". T47D cells were isolated from the parent MCF-7 cells.

Knowing Down ER⁺ Enhances MCF-7 Expression in Yannella Resistant Breast Cancer Cells: It is not known whether ER⁺ and MCF-7 cell proliferation is similar to the parent MCF-7. Prolonged treatment of tamoxifen resistant cells shows an increase in MCF-7 expression.

Transcriptional Regulation Between MCF-7 and ER⁺: Previously, it was reported that pS2 negatively regulates MCF-7 in breast cancer cells. Therefore, we addressed whether O⁶-BG inhibits MCF-7 expression and whether O⁶-BG inhibits ER⁺ expression. ER⁺ cells were treated with either 200 nM or 100 nM O⁶-BG or tamoxifen. ER⁺ expression was consistently increased in T47D breast cells with different concentrations of O⁶-BG and tamoxifen (Fig. 1A,B). The tamoxifen treated cells showed that ER⁺ expression is independent of the drug combination in normal breast cancer cells (Fig. 1C).

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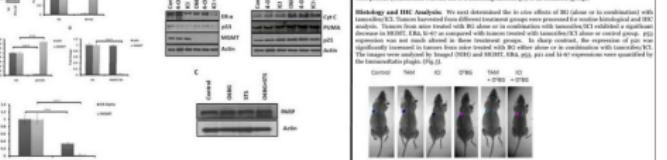


Figure 2: ER⁺ expression remains O⁶-BG resistant. ER⁺ breast cancer cells were treated with 100 nM O⁶-BG for 72 h and 200 nM for 48 h and then harvested for total RNA extraction. ER⁺ protein was analyzed by Western blotting. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG for 72 h and 48 h and then harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot.



Figure 3: ER⁺ breast cancer T47D cells were treated with 0, 100 nM or 200 nM O⁶-BG alone or 0, 100 nM or 200 nM tamoxifen alone or O⁶-BG + tamoxifen. Cell cycle distribution was determined by PI staining and flow cytometry. Cell cycle distribution is shown for O⁶-BG alone (n=3) and O⁶-BG + tamoxifen (n=3). Proliferation rate was measured by BrdU incorporation assay for 0, 100 nM or 200 nM O⁶-BG alone (n=3) and O⁶-BG + tamoxifen (n=3). Statistical significance was determined by ANOVA.



Figure 4: Yannella resistant MCF-7 cells. Yannella breast cancer cells were treated with 0, 100 nM or 200 nM O⁶-BG alone or 0, 100 nM or 200 nM tamoxifen alone or O⁶-BG + tamoxifen. ER⁺ protein was analyzed by Western blotting. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot.

Figure 5: ER⁺ breast cancer T47D cells were treated with 0, 100 nM or 200 nM O⁶-BG alone or 0, 100 nM or 200 nM tamoxifen alone or O⁶-BG + tamoxifen. ER⁺ protein was analyzed by Western blotting. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot.



Figure 6: ER⁺ breast cancer T47D cells treated with O⁶-BG + tamoxifen. ER⁺ breast cancer T47D cells were treated with 0, 100 nM or 200 nM O⁶-BG alone or 0, 100 nM or 200 nM tamoxifen alone or O⁶-BG + tamoxifen. ER⁺ protein was analyzed by Western blotting. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot.



Figure 7: ER⁺ breast cancer T47D cells were treated with 0, 100 nM or 200 nM O⁶-BG alone or 0, 100 nM or 200 nM tamoxifen alone or O⁶-BG + tamoxifen. Cell cycle distribution was determined by PI staining and flow cytometry. Cell cycle distribution is shown for O⁶-BG alone (n=3) and O⁶-BG + tamoxifen (n=3). Proliferation rate was measured by BrdU incorporation assay for 0, 100 nM or 200 nM O⁶-BG alone (n=3) and O⁶-BG + tamoxifen (n=3). Statistical significance was determined by ANOVA.

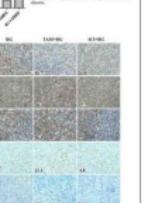


Figure 8: Yannella resistant MCF-7 cells. Yannella breast cancer cells were treated with 0, 100 nM or 200 nM O⁶-BG alone or 0, 100 nM or 200 nM tamoxifen alone or O⁶-BG + tamoxifen. ER⁺ protein was analyzed by Western blotting. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot. ER⁺ cells were treated with 100 nM or 200 nM O⁶-BG or tamoxifen and harvested for total RNA extraction. ER⁺ protein was also extracted from ER⁺ cells treated with tamoxifen and analyzed by Western blot.

Conclusions

1. In the present study, we observe that O⁶-BG plus tamoxifen is more effective than O⁶-BG alone in the reduction of ER⁺ and pS2 expression.
2. Dose-reduction of O⁶-BG by tamoxifen breast cancer cells to avoid side effects.
3. We observed that combination therapy of O⁶-BG and tamoxifen might enhance the effectiveness of O⁶-BG in tamoxifen resistant cells.
4. Combination therapy of O⁶-BG and tamoxifen is effective in tamoxifen resistant cells.

Acknowledgements

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Bad example 1


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O⁶-Benzylguanine Inhibits Tamoxifen Resistant Breast Cancer Cell Growth and Resensitizes Breast Cancer Cells to Anti-Estrogen Therapy

Joshua Smith*, George C Bobust*, Rafael Madero-Vishal*, Jimmie Colon*, Beth Isley*, Jonathan Tick*, Kalkunte S. Srivinugopal and Santi Konduri*

*Cancer Research Institute of M.D Anderson Cancer Center Orlando *Texas Tech University Health Sciences Center, Amarillo, TX

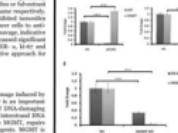
Abstract

Endocrine therapies using antagonists are best used for breast cancer, however, tumor resistance to tamoxifen remains a stumbling block for successful therapy. Based on our recent study on the development of the DNA repair mechanism induced by tamoxifen resistance, we hypothesized that the mechanism for tamoxifen resistance may be due to increased expression of the DNA repair enzyme O⁶-benzylguanine methyltransferase (BMG) at a non-tumor specific site (breast). We report here that tamoxifen resistant breast cancer cells overexpress BMG and that it is overexpressed in tamoxifen resistant cells and tissues.

Posters rarely need abstracts

Introduction
Recent advances in breast cancer research have identified key pathways involved in the repair of DNA damage induced by chemotherapy agents. The ability of cancer cells to repair genetic DNA damage and inhibit DCLR repair is an important mechanism to ensure tumor progression. Our previous work has shown that tamoxifen induces the expression of O⁶-benzylguanine alkylating agent attack the indispensable 3' position on DNA. Tamoxifen induces and highly contributes increased BMG expression in breast cancer cells and tissues. When tamoxifen is administered alone or in combination with doxorubicin or cisplatin, whereas tamoxifen alone increased and decreased tamoxifen resistance significantly. BMG inhibited tamoxifen-induced apoptosis in breast cancer cells. These findings indicate that BMG may play a role in modulating the anti-tumor effects of tamoxifen against breast cancer cells. This combination also enhanced the cyclin E/cdk4 and cyclin D/cdk4 complex to increase cell cycle progression. BMG inhibited the expression of ER^α, ER^β and tamoxifen resistance in breast cancer cells. Thus, tamoxifen and BMG may be an effective approach for overcoming tamoxifen resistance.

Text dissolves into intimidating, boring gray

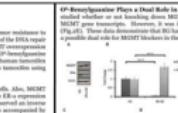

Too small and too much


Results
Prolonged Treatment of Tamoxifen Increases MDM2 Expression: We developed a tamoxifen resistant MCF-7 cell line by serial treatment of tamoxifen for 10 months. As shown in Figure 1, MCF-7 cells on line 3 (MCF-T) produced significantly more MDM2 mRNA and protein levels than the parental MCF-7. Prolonged treatment of tamoxifen resistance leads to MDM2 overexpression in breast cancer cells. Therefore, whether the ER^α is involved in induction of MDM2 expression has to be determined.

Knocking Down ER^α Enhances MDM2 Expression in Tamoxifen Resistant Breast Cancer Cells: It is not known whether ER^α and MDM2 transactivates each other. To test this hypothesis, we examined whether down regulation of ER^α has any effect on endogenous MDM2 expression in these cells. The result showed that knockdown of ER^α significantly reduced MDM2 mRNA and protein levels in these cells. Western blot analysis was performed and the reduction of ER^α protein levels in these cells. Western blot analysis of ER^β protein expression in tamoxifen resistant and normal MCF-7 cells, Interestingly, the results in the right panel of Figure 2 show that ER^β expression is increased in tamoxifen resistant cells. This suggests that ER^β may have a role in tamoxifen resistance. Therefore, the results suggest that ER^β mediated signaling function can response greater gene expression in these cells.

Transcriptional Regulation Between MDM2 and p21: Previously, it was reported that p21 specifically regulates MDM2 in breast cancer cells. Therefore, we addressed whether p21 may regulate MDM2 expression. We report that tamoxifen treatment significantly induced MDM2 mRNA and protein expression in tamoxifen resistant cells, whereas p21 mRNA and protein expression was moderately increased in tamoxifen resistant cells with different expression patterns. In addition, tamoxifen treatment significantly induced the expression of MDM2 in tamoxifen resistant MCF-7 cells whereas p21 mRNA levels were unaffected in MCF-T cells (Figure 3). These results confirm that p21 can regulate MDM2 at the transcriptional level.

Too small and too much

Crammed!


Caption not aligned with figure

Figure 1. MCF-7 parent and tamoxifen resistant MCF-T cells were treated with tamoxifen for 10 months. Total RNA was isolated from these cells and Northern blot analysis was done to analyze the expression of MDM2 and p21 in these cells. The figure clearly shows that MDM2 mRNA and protein expression was significantly increased in tamoxifen resistant MCF-T cells compared to the parental MCF-7 cells.

Figure 2. Tamoxifen increases MDM2 basal expression. MCF-7 cells were transduced with vector or clones of ER^α or ER^β and tamoxifen resistant MCF-T cells were transduced with vector or clones of ER^α or ER^β for 10 months. Total RNA was isolated from these cells and Northern blot analysis was done to analyze the expression of MDM2 and p21 in these cells. The results clearly show that MDM2 expression was significantly increased in tamoxifen resistant MCF-T cells.

Figure 3. MDM2 basal expression was significantly increased in tamoxifen resistant MCF-T cells. Total RNA was isolated from these cells and Northern blot analysis was done to analyze the expression of MDM2 and p21 in these cells. The results clearly show that MDM2 expression was significantly increased in tamoxifen resistant MCF-T cells.

Crammed!

Conclusions
In the present study, we determine that prolonged treatment of tamoxifen increases drug resistance by inducing the DNA repair protein O⁶-benzylguanine methyltransferase (BMG). Therefore, the expression of BMG is involved in tamoxifen resistance. By knocking down these cells to anti-estrogen resistance, we found that tamoxifen resistance was significantly reduced. Our results further supported that combination therapy of anti-estrogen and BMG may not only sensitize these cells to tamoxifen but also decrease the expression of anti-estrogen receptor genes. Therefore, decreasing estrogen receptor expression and increase tamoxifen sensitivity will be a useful strategy for improving the therapeutic efficacy of tamoxifen.

Acknowledgements

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Methods Training (English)

Bad example 2

Judge a catalyst by its anions rather than by its ligands

"Judge a man by his questions rather than by his answers." — Voltaire

Luca Biasiolo
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supervisor: Daniela Zuccaccia
GuruRank: Love for design

Introduction

Heterogeneous gold catalysis is a hot growing area in organometallic chemistry (Chem Rev 2007, 107, 5065) and it's received increasing attention. In a brief unpolished term it is generally mentioned that the ligand environment around the gold center affects the reaction outcome, while the anion environment around the gold center influences the reaction rate. However, there are more subtle effects influencing yields (such as steric hindrance, electron density, electron-withdrawing character, etc.) and the reaction mechanism. Therefore, the role of the ligand and anion environment in the reaction mechanism is still under investigation.

DOI: 10.26432/24.3891. In the other hand, also the step after an important one influencing the overall yield is often neglected. We decided to focus our effort on the investigation of the influence of the anion on the reaction mechanism of the reduction of nitroarenes using the same approach and experimental approach.

Figure 1: Reaction scheme showing the reduction of nitroarenes by NaBH₄ in the presence of L-Au-Cl and AgX. The reaction involves the formation of an OSIP intermediate, followed by nucleophilic attack on the nitro group to form Intermediate II.

AIM OF THE PROJECT

The scope of the project (short) of gold-catalyzed reduction of substituted benzene ligands are more effective than gold, and a better understanding of the reaction mechanism is needed. The aim of this work is to study the effect of the anion environment on the reaction mechanism, focusing especially on the role of the ligand and anion environment in the reaction mechanism.

1 OSP structures

Once OSP is reduced the Outer Sphere Ion-Pair that is formed during the reduction cycle. In the first part we observed that the charge (±1) is not placed over the gold, as generally mentioned. Gold could be localized at one of the circles, depending on the same structure.

2 Nucleophilic Attack

From our results, it is evident that the correct choice of L, in order to have a better performance of the gold catalyst, is enough. This may help to apply the innovative thought pattern to other gold-catalyzed reactions of reduced and increased interest. In the second part, we observed that the reaction mechanism is different from what was expected. The reaction mechanism is different from what was expected. The reaction mechanism is different from what was expected.

3 Protodesign

During this stage the most important factors are the choice of L with a low L/Au ratio (which depends also on the ligand properties). The activity versus the weaker reaction sites (L & Au) is increased, and the reaction mechanism is changed. For example, for PhNO₂, complete the best yields are 20% with the reaction mechanism involving the Au(0) center.

Experimental Details

General: All the gold complex were synthesized using the proper silver salts used *in situ* or isolated. These stable complexes were used in the reaction with NaBH₄ in THF/H₂O (10:1 v/v).

For NaBH₄ a suspension of 0.04 g (7.94 mMOL) and 20 mL (Dioxane/Promethanol) was used to dissolution of the Pd. Details: we noted our stability in two model reactions both are related to the reduction of nitroarenes. The entries was dissolved in THF/Promethanol (1:1 v/v).

Works published during the PhD

1. Biasiolo et al., Chem. - Eur. J. 2008, 14, 10840.
2. Biasiolo et al., Chem. Commun. 2008, 12, 2307.
3. Biasiolo et al., Chem. Commun. 2008, 21, 1447.
4. Biasiolo et al., Chem. Commun. 2009, 10, 1047.

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Catalysis Research Center **François Dainton Fellow** **François Dainton Fellow**

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Bad example 2

Judge a catalyst by its anions rather than by its ligands

"Judge a man by his questions rather than by his answers." — Voltaire

Luca Biasiolo
luca.biasiolo@unimi.it
supervisor: Daniela Zuccaccia
Gesamturk! Love for science

Introduction
Homogeneous gold catalysis remains one of the most important areas in organometallic chemistry (Chem Rev 2012, 112, 244). In a homogeneous system it is generally considered that the reaction mechanism is well understood. However, in more demanding reaction spaces (such as more extensive solvents and substrates), an increase in reaction complexity is observed. This is the case for the reaction of a gold complex with a nucleophile (J Am Chem Soc 2012, 134, 5895). On the other hand, also the step after an important rate influencing reaction is not generally well understood. We decided to study our reaction on the reaction mechanism of the second step, in order to gain some insight through our experiments and theoretical approach.

AIM OF THE PROJECT
The scope of the project (theory of gold-catalyzed reactions of unsaturated ketone ligands and nucleophiles) can be divided into two main parts:
1. **OSIP structures**
How OSIP are related to the Outer Sphere Ion Pair that is formed in the reaction cycle. In the first part we observed that the outer sphere ion pair placed over the gold is generally remained. The position of the outer sphere ion pair depends on the same structure.

2. **Nucleophilic Attack**
Role and position of the anion are studied in order to understand what is the RDS. This gives the dissociation mechanism of the outer sphere ion pair. One of the other side reactions of gold-catalyzed reactions is the reduction of the NHC. Our results show that the NHC must be reduced in order to be a potential nucleophile.

Protodesorption
During this step the most important factors are the identity of P^+ with L^+ and Au^{+2} that depends on the reaction conditions. The activity versus the reaction conditions is shown in the figure below. The reaction conditions are P^+ , Au^{+2} , NHC and H_2O . The reaction time is 10 min . The reaction is carried out at 50°C and $\text{pH} = 7$. The reaction is monitored with UV-vis spectroscopy with $\lambda = 350 \text{ nm}$.

Experimental Details
General: All the gold complex were synthesized using the proper silver salts used *in situ* or isolated. These silver salts were used to reduce the gold salt to the gold complex. The reaction was carried out in CHCl_3 and CH_2Cl_2 .
In: Au^{+2} in CHCl_3 solution (10 mM HgCl₂) and 20% (v/v) CH_2Cl_2 .
Details: we added the substrate in two mole reactions both are equal (relative to gold complex). The anion was dissolved in CH_2Cl_2 and H_2O .

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Works presented during:

- 1. Biasiolo et al., Chem. Mater. 2012, 24, 5895.
- 2. Biasiolo et al., J Am Chem Soc 2012, 134, 5895.
- 3. Biasiolo et al., J Am Chem Soc 2012, 134, 5895.
- 4. Biasiolo et al., J Am Chem Soc 2012, 134, 5895.
- 5. Biasiolo et al., J Am Chem Soc 2012, 134, 5895.

CONCLUSIONS
From our results, we can see that the correct choice of P^+ in order to get a good catalytic activity is very important. The best choice is the one that has a higher affinity towards the gold. Also the NHC is a very important factor in the reaction. The NHC must be reduced in order to be a potential nucleophile. The reaction mechanism is shown in the figure above.

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Creative example 1

Forecasting a Deep Sea Oil Spill

Water and Oceans

Ryan Gilchrist¹, Robert Hall¹, John Bacon²,
Jon Rees¹, Karen Heywood¹

1: University of East Anglia, Norwich, Norfolk, NR4 7TJ
2: Centre for Environmental, Fisheries and Aquaculture Science (Cefas)

The Faroe-Shetland Channel (FSC) is the primary location for future oil and gas exploration in the UK

Subsurface Spill Dynamics

Deep Sea Spill Stages

1. Blowout
2. Jet Phase
3. Entrainment
4. Plume Phase
5. Trapping
6. Droplet Phase
7. Surfacing
8. Plugged

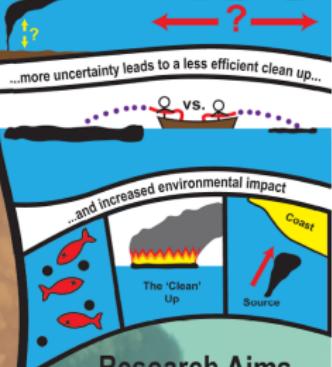
Areas of Uncertainty

What influence does stratification have on the depth in which pollutant trapping occurs?

How does the complex circulation within the channel influence oil trajectory and fate?

Do mesoscale eddies enhance or inhibit water entrainment and oil dispersion?

Small uncertainties will grow over time...



Research Aims

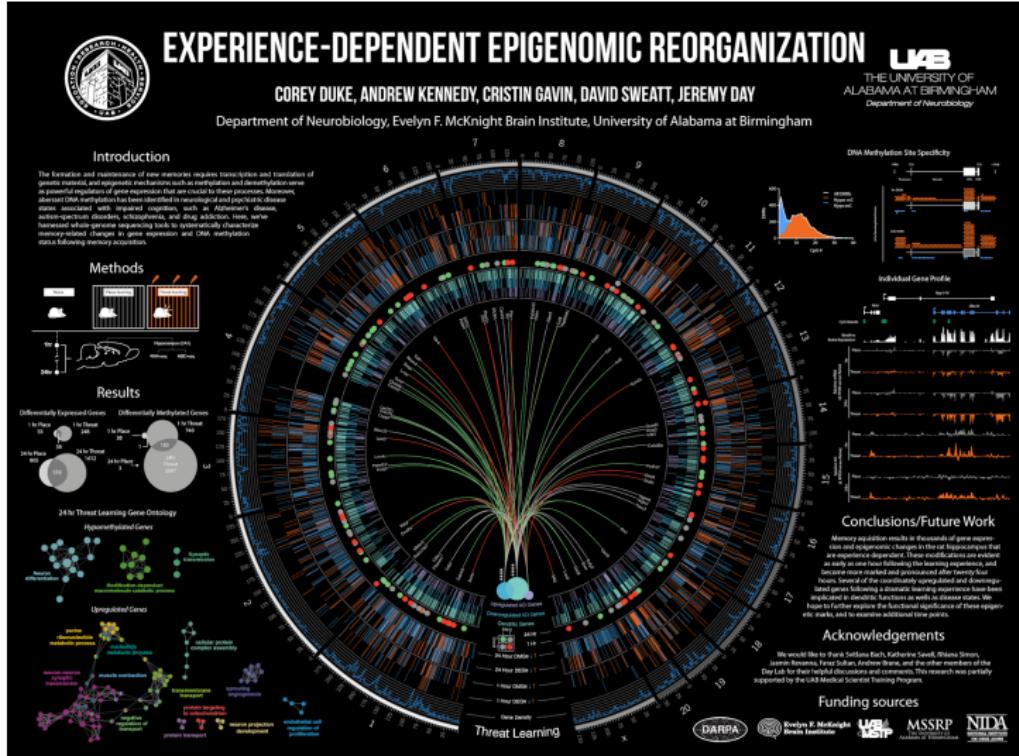
A To benefit the UK industry by reducing the costs and uncertainty involved in producing pollution emergency plans

B To reduce environmental impact by better forecasting the trajectory of a deep sea spill

C To further our understanding of how a deep sea oil spill behaves within a complex oceanographic environment



Creative example 2

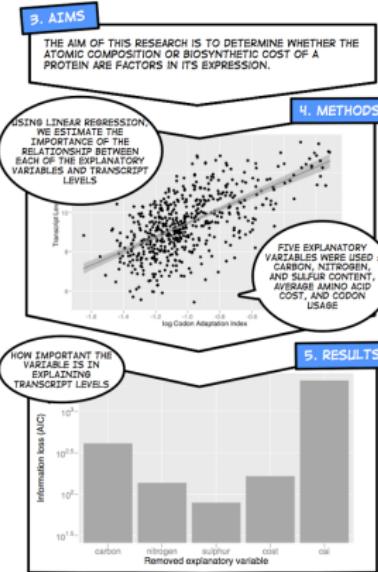
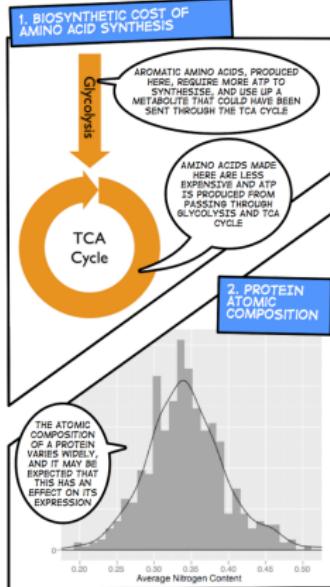


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Creative example 3

PROTEIN BIOSYNTHETIC COST AND ATOMIC COMPOSITION AS PREDICTORS OF GENE EXPRESSION

MICHAEL BARTON, CASEY BERGMAN, DANIELA DELNERI, MAGNUS RATTRAY, STEVE OLIVER



6. CONCLUSIONS

OUR INITIAL ANALYSIS INDICATES THAT BIOSYNTHETIC COST AND ATOMIC COMPOSITION OF A PROTEIN DO MAKE A ROLE IN ITS EXPRESSION, HOWEVER THIS IS VERY SMALL WHEN COMPARED TO OTHER FACTORS SUCH AS CODON USAGE.

OUR FUTURE WORK WILL EXAMINE WHETHER THESE FACTORS PLAY A ROLE IN THE EVOLUTION OF A PROTEIN ACROSS SPECIES, AS WELL AS WHETHER THESE EFFECTS ARE IMPORTANT AT THE METABOLIC LEVEL.

7. OPEN NOTEBOOK SCIENCE

Very rough first draft of background information on protein expression.

ALL THE RESULTS AND ANALYSES OF THIS EXPERIMENT ARE AVAILABLE ONLINE.

THE AIM IS TO PROVOKE WIDER ACCESS AND COLLABORATION.

WWW.MICHAELBARTON.ME.UK

DATA SOURCE

THE DATA USED IN THIS ANALYSIS COMES FROM A YEAST CODON ADAPTATION EXPERIMENT, CASTRILLO ET AL. 2007.

FUNDING

NATIONAL ENVIRONMENT RESEARCH COUNCIL

<http://betterposters.blogspot.de>

Good example 1



Using a Water Balance Model to Bound Potential Irrigation Development in the Upper Blue Nile Basin



Paper Number: GC43C-1178

Anjuli Jain Figueroa¹ - ajainf@mit.edu

Dennis McLaughlin¹ - dennism@mit.edu

¹Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA

1. Introduction

The development of the Grand Ethiopian Renaissance Dam (GERD) on the Nile River has prompted concerns regarding the dam's downstream impact.

The dam is intended for power production, but Ethiopia has a strong food-security incentive to also use it for irrigation.

2. Research Questions

This study sought to explore:

- The limitations on food production in the Upper Blue Nile Basin in Ethiopia.
- The maximum water withdrawal from expanded irrigation of current prominent crops.

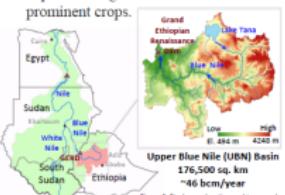


Figure 1: Study area location and topography

3. Method

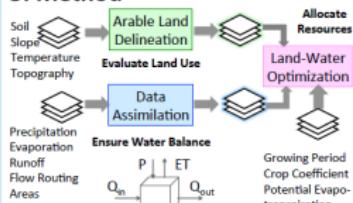


Figure 2: Overview of 3-phase method

4a. Results

Question: Is Ethiopia's food security limited only by water?

Result: 25% of land is suitable for irrigation based on slope, soil and temperature. When water availability is included, this drops to 11% of land.

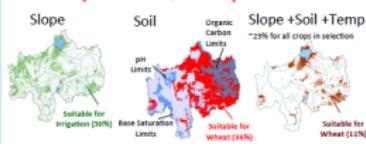


Figure 3: Example of arable land delineation for wheat.

4b. Results

Question: How much water (max.) can be withdrawn for irrigation in the UBN basin?

Result: 3.75 bcm/year - small downstream effect with increased crops.

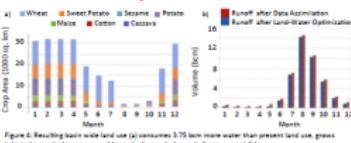


Figure 4: Resulting basin wide land use (a) consumes 3.75 bcm more water than present land use, grows irrigated crops in dry season, and leaves hydrograph shape similar to current (b).

5. Conclusion

A water consumptive land use, which assumes expansion of current dominant crops and no additional land investment (i.e., fertilizers), reduces annual runoff from 46.4 to 42.7 bcm (8% decrease).

There is a possible win-win situation to enhance Ethiopia's food security (currently withdrawing 5 bcm/year) without affecting the flow downstream too severely.

Related Publication

Almeida, M. A., Jain Figueroa, D. B., McLaughlin, and T. A. Elshakry (2016). Extraction of evaporation over the upper Blue Nile basin by combining observations from satellites and river flow gauges. *Water Resources Research*, 52, 644–659, doi:10.1002/2013WR017251.



American Geophysical Union (AGU) Fall Meeting, San Francisco 2018

<http://betterposters.blogspot.de>

Good example 2



Ian Haydon¹, Cathleen Zeymer², Adrian Bunzel², Yakov Kipnis¹, Tom Linsky¹, Po-Ssu Huang³, Don Hilvert², David Baker¹



Designing enzymes from scratch

1. University of Washington

2. ETH Zürich

3. Stanford University

Introduction

Enzymes are capable of accelerating chemical reactions up to 10^{13} times faster than in the absence of catalyst. This astonishing rate enhancement depends, above all, on the preorganization of a precise electrostatic environment within the active site of an enzyme which serves to stabilize the high-energy transition state(s) of a reaction.

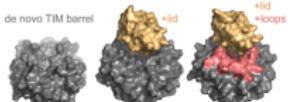
Though a small number of enzymes have successfully been designed by rationally mutating existing proteins, none has shown levels of rate enhancement comparable to a natural, evolved enzyme.

Key limitations include:

1. A general inability to design preorganized active sites
2. Mutational intolerance of natural protein scaffolds
3. Possible errors in modeling the new reaction mechanism

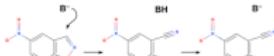
New architectures for enzyme design

For the first time, Rosetta designed proteins can be used in the enzyme design process. These scaffolds are highly thermostable (T_m 70–90°C) and mutationally tolerant,



Kemp elimination – a model reaction

Kemp elimination is a well characterized ring opening reaction wherein a catalytic base extracts a hydrogen from carbon, breaking the N–O bond in benzoxazoles.



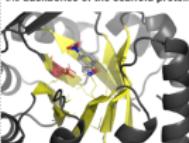
Though the reaction is exothermic, it involves a high energy transition state and is thus considered a model reaction for studying enzyme-catalyzed proton transfer.

Enzyme design workflow using Rosetta

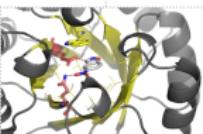
Design begins with a description of all atoms thought to be involved in stabilizing the TS. This collection of disembodied atoms is known as a "theozyme".

This simple theozyme consists of the ligand, a catalytic asp/gl, an optional stabilizing asp/gln, and distance / angle constraints.

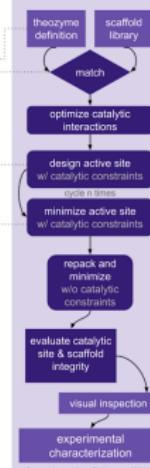
The Matcher algorithm attempts to fit the residues defined in the theozyme into the backbones of the scaffold proteins.



Once in place, the Packer fills in missing side chains, creating an active site with high shape complementarity to the ligand.



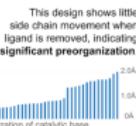
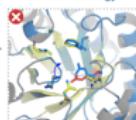
For a subset of designs, the Packer was modified to place specific side chains intended to improve ligand binding/selectivity.



Selecting the best designs in silico

To evaluate the extent of preorganization in each designed active site, the ligand is computationally removed and the active site is allowed to repack and minimize in energy.

This design shows poor preorganization, as the catalytic base adopts an alternative rotamer in the absence of ligand.



Designs are selected based on 1) preorganization of the entire active site 2) agreement with theozyme constraints 3) overall scaffold integrity 4) minimal number of mutations.

Future work

Genes encoding the 40 best Kemp eliminase designs are being synthesized. All designs will be purified and tested using a plate-based fluorescence activity assay. Designs which show detectable levels of activity will be optimized via directed evolution (at ETH Zürich).

For more complex non-model reactions, more complex theozymes are needed. As the complexity of a theozyme file increases linearly, the likelihood of the Matcher finding a suitable scaffold in the PDB drops exponentially. It is for this reason that designed protein scaffolds are needed. A pipeline for producing diverse libraries of de novo TIM barrel scaffolds is being developed.

INSTITUTE FOR
Protein Design
UNIVERSITY OF WASHINGTON

Wissner-Silvika Foundation
ETH zürich

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Methods Training (English)

Good example 3

Cloning, expression and characterization of GH10 xylanases from landfill leachate bacteria *Paenibacillus* sp. MAEPY2

Patric Chua^{1*}, Gary A Dykes², Lee Sui Mae¹

¹ School of Biotechnology, Monash University, Malaysia
² School of Public Health, Curtin University, Australia
*Corresponding author e-mail: tchua@biotech.monash.edu

Background

Landfill wastes are valuable materials with plant biomass, e.g. food/organic wastes, papers and their byproducts.

Major components in plant biomass can be degraded rapidly by the depolymerases and microbials in landfills.

Plant biomass-degrading microbials can be exploited for applications in various industrial processes.

BioProspecting

Landfill leachate was collected from a local landfill site.

Microbial population in leachate was selected as potential source containing cellulase.

Isolate that were resistant to xylanase and cellulase was isolated and identified as *Paenibacillus*: MAEPY2 and MAEPY1.

Xylanase activity of both isolates further tested against other plant cell wall components. Activity against xylan was the highest in MAEPY2.

Xylanase activity of crude enzyme extract was determined against commercial enzymes. Results indicate great potential.

Sequencing

Whole genome of *Paenibacillus* sp. MAEPY2 was sequenced using Illumina HiSeq 2000. The sequencing data was registered in NCBI Genbank under the accession number: MZVQ000000000000.

101 of the open reading frames (ORFs) were annotated as putative enzymes.

249 uncharacterized genes were annotated as putative cellulases.

63% of the 685 ORFs had active cellulase or xylanase activities.

Enzyme studies

Optimum temperature and pH were determined as optimum activity versus activity versus time.

Optimum temperature was determined at 40°C for MAEPY2 and MAEPY1.

Optimum pH was determined at 5.5 for MAEPY2 and MAEPY1.

Figure 1. Effect of temperature and pH on enzyme activity. Enzyme activity was measured at 40°C for MAEPY2 and MAEPY1. Optimum activity was determined at 40°C for MAEPY2 and MAEPY1. Optimum pH was determined at 5.5 for MAEPY2 and MAEPY1.

Cloning and expression

Xyn1 and Xyn2 genes were cloned into pET28A with E. coli host and expressed in BL21 (DE3) host cells.

Expression of Xyn1 and Xyn2 genes in BL21 (DE3) host cells was induced using Inducer (IPTG) and overnight induction at 30°C.

Purification was performed for the N-terminal Xyn1 and Xyn2 using AKTA Purifier (GE Healthcare).

SDS-PAGE was performed using Laemmli's method¹. A native-PAGE was performed for xylanose specificity.

Figure 2. Native-PAGE and zymogram analysis of the purified enzymes. Native-PAGE analysis of the purified enzymes showed two distinct protein bands corresponding to Xyn1 and Xyn2.

In this study

We characterized two xylanase genes from *Paenibacillus*, MAEPY2.

Both enzymes have optimum temperature of 30°C to 40°C. Inducer at 40°C, Xyn1 is active at pH 4 to 7, while Xyn2 is active at pH 5 to 7.

SDS-PAGE

A more detailed account of the xylanase-substrate specificity of MAEPY2 and MAEPY1 predicts their synergies/antagonies.

Please take our survey
Leave your comments here
Leave your contact here

Acknowledgments

Funding for this study was provided by the Monash University Research Grant. Authors would like to thank Dr. Gary A. Dykes for his support in this work. We are grateful to the anonymous reviewers for their useful comments and suggestions during the preparation of this manuscript.

References

1. Bell et al. 2008. JMM December 15.
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3. Lauzon et al. 1995. Microbiology 141: 2351-2359.

Monash University
MALAYSIA

<http://betterposters.blogspot.de>

Methods Training (English)

Good example 3



<http://betterposters.blogspot.de>

Insekten als Indikatoren für Renaturierungserfolge

Vasco Elbrecht (Vasco.Elbrecht@rub.de), Ralph Tollrian & Florian Leese

RUB Ruhr-Universität Bochum, Lehrstuhl für Evolutionsökologie und Biodiversität der Tiere GeneStream



Hintergrund

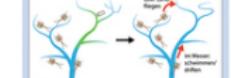
Genetische Veränderungen werden durch europäische renaturierende Maßnahmen auch in Zukunft zu beobachten. Gleichzeitig können diese Veränderungen aufgrund der begrenzten Anzahl von Mütterchen nicht kontinuierlich in der Genpoolrate zurück, wobei nicht klar ist ob:

a) die Renaturierung unterschiedlich war oder

b) die Renaturierung unterschiedliche Genetiken nicht wiederherstellen kann.

Informationen über die Mutationen von empfindlichen Indikatorarten wie z. B. der Fliegenart *Drosophila melanogaster*, sind hilfreich

um den Erfolg von Renaturierungen zu bewerten (Abb. 1).



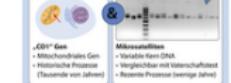
Ziel dieser Masterarbeit war es, das Ausbreitungspotenzial der Art *Drosophila melanogaster* als Indikator für renaturierende Maßnahmen zu überprüfen und mit anderen Methoden zu untersuchen.

Material und Methoden

Die Ausbreitungsfähigkeit und -wege von Insekten können durch verschiedene Methoden untersucht werden. Da Fliegen nicht einzeln gezählt werden, mit modernen molekularen, DNA-basierten Methoden, ist dies jedoch präzise und kostengünstig möglich. Zur Untersuchung wurde die genetische „genetische Fingerabdrücke“-Ausagen zum Zustand und Bestand von Populationen gemacht.



Abbildung 2: Die Drosophila *D. melanogaster*. 214 Fliegen wurden ausgewählt, um die Art im Herkunftsgebiet untersuchen.



Video Poster
Blickt auf die Ergebnisse über die Wiederbesiedlung von ungenutzten Gewässern durch die Fliegenart *Drosophila melanogaster*.



Veröffentlichungen aus der Masterarbeit
Mehr über die Ergebnisse der Masterarbeit und die Methoden der Untersuchung der Fliegenart *Drosophila melanogaster* für die Wiederbesiedlung von Gewässern finden Sie in den folgenden Veröffentlichungen:

Ergebnisse und Diskussion

Analyse des COI-Gens zeigen, dass *D. melanogaster* aus zwei genetisch diversen Gruppen besteht (A und B in Abb. 3). Verschiedene Gruppen sind über das Untersuchungsgebiet relativ gleichmäßig verteilt, was eine gute Fundeuniformität der Individuen zeigt. Die Analyse der hochauflösenden Mitochondriellen Sequenzierung bestätigt, dass alle Populationen genetisch sehr ähnlich sind (Abb. 4).

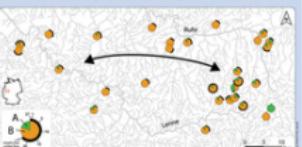


Abbildung 3: Karte des Untersuchungsgebietes mit verschiedenen Populationen. Mit diesem COI-Gen werden zwei genetisch diverse Gruppen bestimmt. Diese Populationen sind über das Untersuchungsgebiet relativ gleichmäßig verteilt, was eine gute Fundeuniformität der Individuen zeigt. Die Analyse der hochauflösenden Mitochondriellen Sequenzierung bestätigt, dass alle Populationen genetisch sehr ähnlich sind (Abb. 4).

-COI und Mitochondrielle Unterschiede zeigen, dass die Populationen genetisch sehr ähnlich sind. Dies bedeutet, dass *D. melanogaster* eine gute Fundeuniformität aufweist.
-Über adulte Fliegenart kann *D. melanogaster* innerhalb weniger Jahre renaturierte Gewässer abschätzen von benachbarten Bächen wiederherstellen.

-Somit eignet sich die Art als guter Indikator, um den Erfolg von Renaturierungen zu überprüfen.

-Diese Arbeit zeigt das Bildungswertige ungenutzte Potenzial genetischer Methoden.

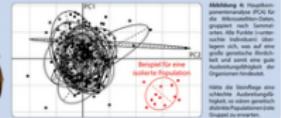


Abbildung 4: Hervorheben der Mitochondriellen PCR-Daten der Populationen. Die Populationen sind in zwei Gruppen unterteilt: eine große Gruppe mit schwarzen Punkten und eine kleinere Gruppe mit roten Punkten. Die Populationen scheinen sich, was auf eine gute Fundeuniformität hindeutet.

Not: die Beobachtung einer lokalen Population ist wichtig, da dies gleichzeitig die Wiederbesiedlung eines Gewässers durch die Fliegenart *Drosophila melanogaster* bestätigt.

Wirtschaftliche Bedeutung

Renaturierungen sind fast immer teuer, jedoch oft nicht direkt erfolgreich. Ohne Wiederbesiedlung an ungenutzten Maßnahmen oder der fehlenden Nähe von Quellpopulationen scheitert, kann ohne Kenntnis über die Ausbreitungsfähigkeit der Arten nicht eindeutig bestimmt werden. Die Fliegenart *Drosophila melanogaster* kann dies.

Auch über die genetische Diversität die Gefährdung von Populationen (und somit auch die Gefährdung ihrer Funktion im Ökosystem) durch anthropogene Einflüsse bestimmt lässt:

- genetische Daten entscheidende Hinweise über die Isolation und Wiederbesiedelbarkeit von Gewässerbereichen geben können,
- anhand von genetischen Landkarten geprägte Stellen mit hoher Wiederbesiedelungspotenzial bestimmt werden können,
- durch schlechte Informationen durch molekulare Methoden mit vergleichsweise geringem Aufwand und kostengünstig genommen werden können.



Über den Autor
Name: Dr. rer. biol. med. Michaela Schäfer
Beruf: Doktorandin im Rahmen der Arbeitsgruppe „Wiederbesiedlung von Gewässern durch Fliegenarten“ am Lehrstuhl für Evolutionsökologie und Biodiversität der Tiere der Ruhr-Universität Bochum.



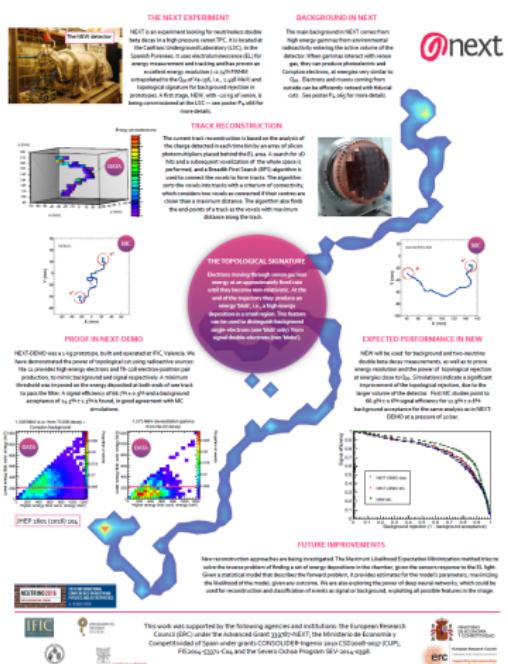
Projektpartner
Dr. rer. biol. med. Michaela Schäfer, Dr. rer. biol. med. Daniel Hering und Martin Sonnenburg
Lehrstuhl für Evolutionsökologie und Biodiversität der Tiere der Ruhr-Universität Bochum.

C. Woolston. Conference presentations: Lead the poster parade.

Improving example 1

Topological signature in the NEXT high pressure xenon TPC

Paola Ferrario, Instituto de Física Corpuscular (Universitat de València-CSIC)
on behalf of the NEXT Collaboration

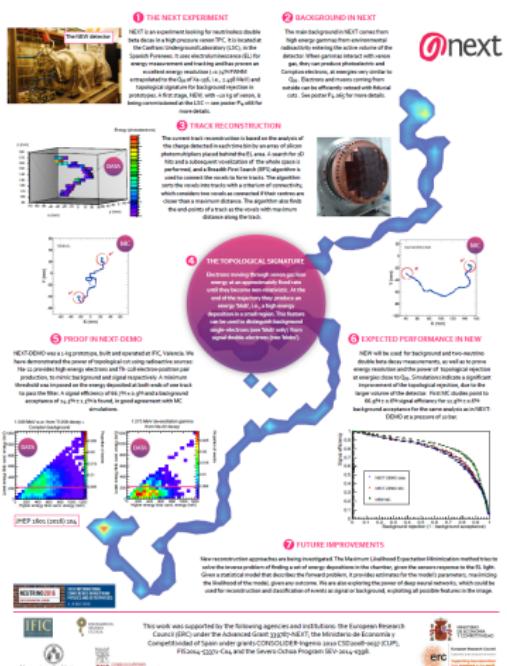


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Improving example 2

Topological signature in the NEXT high pressure xenon TPC

Paola Ferrario, Instituto de Física Corpuscular (Universitat de València-CSIC)
on behalf of the NEXT Collaboration



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H-BRS Examples

- Active Vibration Control of engine mounts -

Determinisation of local temperature without any sensors?

- Student of mechanical engineering at Hochschule Bonn-Rhein-Sieg

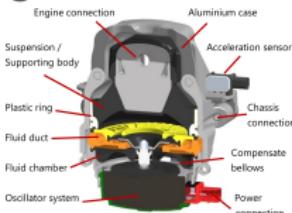
BACKGROUND

Active Vibration Control - Engine Mount

- State of the Art in vibration damping of engine oscillation in vehicles



Assembly / Components



Function

- Measurement of the chassis-side frequency from every mount
- Calculation of the necessary amplitude and phase of the oscillator
- Rheologic damping by the liquid in the fluid duct and tribological damping by the rubber

WANT TO SEE AN ANIMATION OF THE FUNCTION?



References:

Pictures of the engine mount: Internal Documents of Boge Rubber & Plastics GmbH
Theoretical Principles of heat transfer: (CI) • „VDI-Wärmeatlas“ • „Grundlagen der Wärmeübertragung“

ACTUAL MASTER RESEARCH (in progress)

Introduction

The vibration damping of the active engine mount is still satisfactory in a warm driven vehicle. Difficulties arise when starting a cold vehicle because of increasing temperatures of the mount. This problem is even caused in bad weather. The reason can be found in the temperature depending changes of material properties of the mount components. These changes are not considered currently by the algorithm of the control unit.

Rectification can be reached about temperature sensors, but they increase the unit price. Therefore it should be considered to determine the temperature and the conditional change by a calculation regulation.

Aim of the Project

- Development of a calculation regulation to estimate the temperature of the active engine mount
- Identification of the temperature with the greatest influence on vibration damping
- Implementation of the temperature-dependent vibration damping in the control unit

Difficulties / Obstacles

- Time-varying boundary conditions
- Low temperature and vehicle information
 - temperature of environment, coolant and oil
 - velocity
- Unsteady heat conduction of rubber and the fluid
- Low storage capacity of the control unit for the calculate regulation

Alternating Direction Implicit-Method

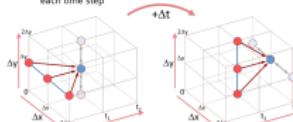
- 2D-Calculation for unsteady heat conduction without internal energy source to solve 3D problems:

$$\frac{\partial \theta}{\partial t} = \pi \left(\frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} + \frac{\partial^2 \theta}{\partial z^2} \right) + \frac{q'''}{p' \cdot C}$$

- Replacement of derivatives by discretization for each direction for example in y-direction:

$$\frac{\theta_{i+1,j}-\theta_{i,j}}{\Delta t} = \frac{(\theta_{i+1,j+1}-\theta_{i+1,j})-(\theta_{i,j+1}-\theta_{i,j})}{(\Delta x)^2} + \frac{(\theta_{i+1,j+1}-\theta_{i,j+1})-(\theta_{i+1,j}-\theta_{i,j})}{(\Delta x)^2}$$

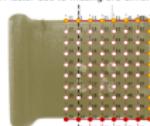
- Calculation of heat conduction in alternating direction for each time step



Temperature behavior of a rubber cube

- Determination of the cooling behavior of a rubber cube under free convection
- Implementation of Neumann and Newtonian boundary conditions
- Expand by a correction factor due to missing 3rd dimension

- Convection
- Heat conduction
- Adiabatic ground
- Symmetry condition

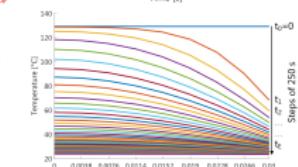
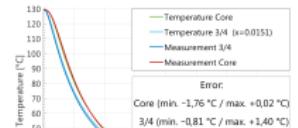


Results / Validation with Measures

- Initial values: - Temperature of rubber cube: 129.1 °C
- Ambient temperature: 23.3 °C

- Discretisation of 9x9 points, correction factor = 3.25

Temporal temperature curves



Conclusion

- Good results for further simulations of the mount
- Fast calculation up to ≈ 4,983 seconds for entire time
- Difficult to adapt for complex geometries



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http://xing.to/[REDACTED]



Hochschule
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University of Applied Sciences

B BOGE
RUBBER & PLASTICS

- Active Vibration Control of engine mounts -

Determinisation of local temperature without any sensors?

- Student of mechanical engineering at Hochschule Bonn-Rhein-Sieg

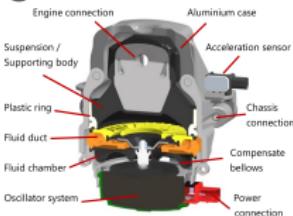
BACKGROUND

Active Vibration Control - Engine Mount

- State of the Art: vibration damping of engine oscillation in vehicles



Assembly / Components



Function

- Measurement of the chassis-side frequency from every mount
- Calculation of the necessary amplitude and phase of the oscillator
- Rheologic damping by the liquid in the fluid duct and tribological damping by the rubber

WANT TO SEE AN ANIMATION OF THE FUNCTION?



ACTUAL MASTER RESEARCH (in progress)

Introduction

The vibration damping of the active engine mount is still satisfactory in a warm driven vehicle. Difficulties arise when starting a cold vehicle because of increasing temperatures of the mount. This problem is even caused in bad weather. The reason can be found in the temperature depending changes of material properties of the mount components. These changes are not considered currently by the algorithm of the control unit.

Rectification can be reached about temperature sensors, but they increase the unit price. Therefore it should be considered to determine the temperature and the conditional change by a calculation regulation.

Aim of the Project

- Development of a calculation regulation to estimate the temperature of the active engine mount
- Identification of the temperature with the greatest influence on vibration damping
- Implementation of the temperature-dependent vibration damping in the control unit

Difficulties / Obstacles

- Time-varying boundary conditions
- Low temperature and vehicle information
 - temperature of environment, coolant and oil
 - velocity
- Unsteady heat conduction of rubber and the fluid
- Low storage capacity of the control unit for the calculate regulation

Alternating Direction Implicit-Method

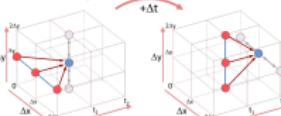
2D-Calculation for unsteady heat conduction without internal energy source to solve following formula:

$$\frac{\partial \theta}{\partial t} = \pi \left(\frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} + \frac{\partial^2 \theta}{\partial z^2} \right) + \frac{q'''}{p' C}$$

• Replacement of derivatives by discretization for each direction for example in y-direction:

$$\frac{\theta_{i+1,j}-\theta_i}{\Delta t} = \pi \left(\frac{\theta_{i+1,j+1}-2\theta_{i+1,j}+\theta_{i+1,j-1}}{(\Delta y)^2} + \frac{\theta_{i,j+1}-2\theta_{i,j}+\theta_{i,j-1}}{(\Delta x)^2} \right)_i$$

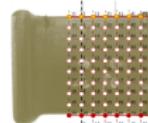
• Calculation of heat conduction in alternating direction for each time step



Temperature behavior of a rubber cube

- Determination of the cooling behavior of a rubber cube under free convection
- Implementation of Neumann and Newtonian boundary conditions
- Expand by a correction factor due to missing 3rd dimension

- Convection
- Heat conduction
- Adiabatic ground
- Symmetry condition

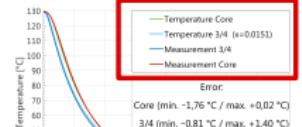


Results / Validation with Measures

- Initial values: - Temperature of rubber cube 129.1 °C
- Ambient temperature 23.3 °C

- Discretisation of 9x9 points, correction factor = 3.25

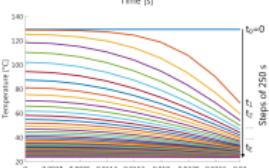
Temporal temperature curves



Error:

Core (min. -1.76 °C / max. +0.02 °C)

3/4 (min. -0.81 °C / max. +1.40 °C)



Conclusion

- Good results for further simulations of the mount
- Fast calculation up to ≈4,983 seconds for entire time
- Difficult to adapt for complex geometric

References:

Pictures of the engine mount: Internal Documents of BOGE Rubber & Plastics GmbH
Theoretical Principles of heat transfer: (CI) • „VDI-Wärmeatlas“ • „Grundlagen der Wärmeübertragung“



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BOGE
RUBBER & PLASTICS

METAL HYDRIDE STORAGES AS PART OF A *GREEN* FUTURE



Dr. Nils Bornemann², Prof. Dr. Dirk Reith¹



Background

Global demand for energy is steadily increasing. Hydrogen with its high energy-weight ratio offers a valuable alternative solution to both save and transport energy. Therefore hydrogen is an interesting option for new mobile alternative drivelines and makes emission-free combustion possible. Hydrogen can be stored in chemical form in metal hydride storages, which offer considerable benefits such as high storage density of hydrogen at a low pressure compared to pressure tanks. Nevertheless, the main problem is to manage the thermal activities inside a metal hydride storage.



Reaction kinetics

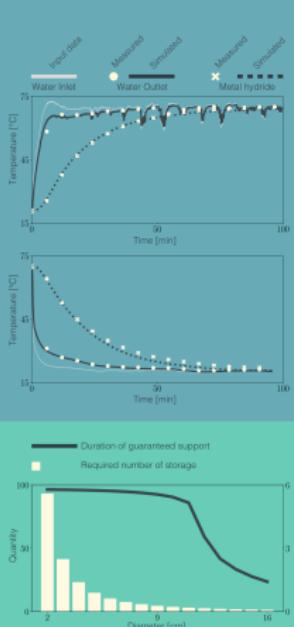
Metal hydride is fundamentally a chemical connection between hydrogen and a metal alloy. This process deposits hydrogen atoms inside the metal lattice so that a new phase is created called metal hydride. The outcome of this process (desorption/absorption) is influenced by the increase or decrease of heat. Firstly, thermal energy is generated due to desorption. Secondly, the released heat is needed to cause a desorption of hydrogen. Adequate heat management is essential to control these thermal activities.



Hochschule Bonn-Rhein-Sieg Hochschule Bonn-Rhein-Sieg



DAW Stahl Metall Engineering GmbH



References:

1. Mokarramabadi S.S. et al. International Journal of Hydrogen Energy 41 (2016) 3470-3484
2. Jiang and Shi, Journal of Computational Physics 128, 252-261 (1996)
3. Multakumar P. et al. Journal of Alloys and Compounds 472 (2009) 466-472



Application Structure



An electrical engine requires energy which is supplied in this case by hydrogen. However, the chemical energy contained in hydrogen has to be electrochemically converted into electrical power. As an energy converter, the fuel cell makes emission free combustion and generation of electrical power using hydrogen possible. The hydrogen is stored inside a metal hydride storage. Due to the considerable heat needed and/or produced, a heat management component is also essential. Heat is created in the fuel cell. During the discharge of the metal hydride storage, the heat produced in the fuel cell is transferred to the storage.



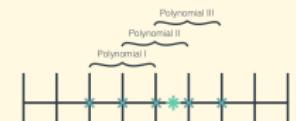
Numerics (WENO scheme)

A weighted essentially non-oscillatory scheme is implemented to obtain a value for half nodes. This procedure avoids numerical oscillations. In addition, WENO schemes achieve a high level of accuracy. The half node value is interpolated by 3 different polynomials. These polynomials are weighted according to their smoothness and form a linear combination. These half node values are then used for difference quotients to estimate the derivatives.



Partial differential equations

$$\begin{aligned} &\text{Energy conservation: } \frac{\partial T}{\partial t} = JF(FT) - \dot{H}_{\text{reaction}} \Delta H \\ &\text{Momentum conservation: } \frac{du}{dt} = -Fp + \mu T(P_{\text{ext}}) - u \cdot \nabla u + H_D \\ &\text{Mass conservation: } \frac{\partial \rho}{\partial t} = -\nabla(\rho u)_D - \dot{H}_{\text{reaction}} - \dot{H}_{\text{value}} \end{aligned}$$



Further steps

- Determining the reaction kinetics properties of FeTiMg such as enthalpy, entropy and reaction constants.
- Simulation model and an economic balance sheet of a dynamic mobile application such as a fork lift truck and/or a ferry.
- Search for other possible applications where hydrogen is an essential part.

Acknowledgement:

I would like to express my gratitude to my mentor Dr. Nils Bornemann as well as my mentor Prof. Dr. Dirk Reith who gave me the opportunity to do this project. Secondly, I would like also to thank Prof. Dr. Oerd Steinbach, Bettina Neumann, Thomas Schupp, Dr. Markus Schneider and Markus Lutz for answering my questions.

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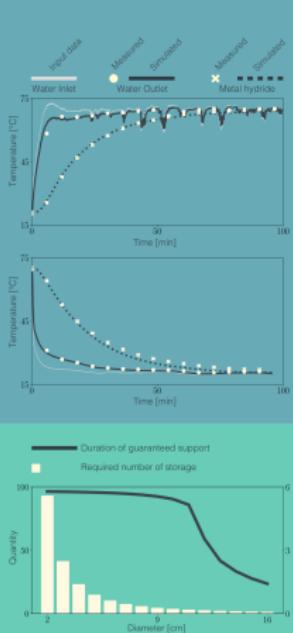
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No Research Questions or Hypothesis



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References:

1. Muthukrishnan S.S. et al. International Journal of Hydrogen Energy, 41 (2016) 3470-3484
2. Jiang and Shi, Journal of Computational Physics, 128, 222-239 (1996)
3. Mukhopadhyay P. et al. Journal of Alloys and Compounds, 472 (2009) 468-472



No clear workflow logic

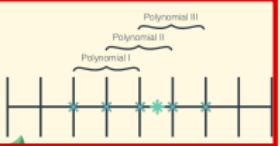
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$$\text{Mass conservation: } \frac{\partial \rho_{\text{H}_2}}{\partial t} = -F(\rho_{\text{H}_2} V_{\text{ext}}) - \dot{H}_{\text{reaction}} - \dot{H}_{\text{value}}$$

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Optimization of force field parameters for molecular simulations

1 - Introduction

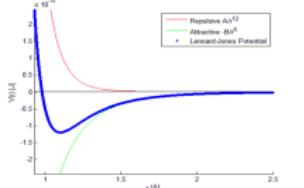
The importance of molecular simulations regarding the development of new materials, medical components and more efficient chemical processes is rising. Besides providing insight in thermodynamical and chemical properties, experiments can be time consuming or time consuming experiments can **partly be replaced by simulations**. This saves resources such as substances, time and money.

Developing models for molecules consists of designing and optimizing mathematical functions (potentials) describing the interactions between atoms within a molecule (bonded interactions) and more complicated, separate attractions and repulsions. The collection of potentials used in a molecular simulation is called **force field**. To adapt the force field to different types of atoms and molecules the **potentials are parameterized**.

The optimization aims for a set of parameters, so that the molecular behaviour and physical properties in the simulation reproduce experimental data.

2 - Parameters

This study focuses on the **Lennard-Jones parameters σ and ϵ** , which are used for the modeling of **inter-molecular interactions** (i.e. interactions between multiple molecules). The Lennard-Jones Potential is composed of an attractive and a repulsive component as a function of the distance between the particles (see $V(r)$ in the figure below).



3 - Optimization

The **Lennard-Jones parameters σ and ϵ** must be chosen such that the simulation results agree with target data. Here the target data consists of experimentally determined **bulk-phase density** (i.e. a macro-scale property) and **internal conformational energies** [1] (i.e. a micro-scale property) that are obtained using quantum chemistry calculations.

The **desired result** is a set of parameters, which allows to extract information on both, the atomistic and macroscopic scale, from molecular simulations.

4 - Workflow

There is an existing workflow ("A Gradient-based Optimization Workflow" [2], **GROW**), which allows to optimize force-field parameters. Therefore, a loss function (see Figure 1) minimizes with numerical optimization methods. The optimal set of parameters is represented by a loss-value of 0.

Depicted in the diagram below is the current workflow in **blue**:

- depiction using an user-defined initial set of parameters (with external simulation tool)
- evaluating the results by comparing to target data:
 - next iteration: slightly change parameters and re-simulate
 - ...
 - final set of parameters

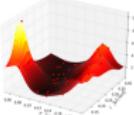
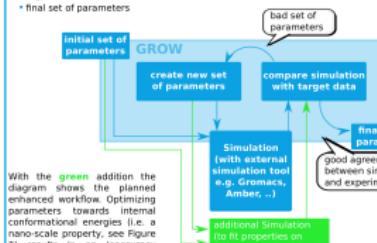


Figure 1: loss function



With the **green addition** the diagram shows the planned enhanced workflow. Optimizing parameters towards internal conformational energies (i.e. a nano-scale property, see Figure 2) results in an inaccuracy regarding the density (i.e. a macro-scale property, see Figure 3).

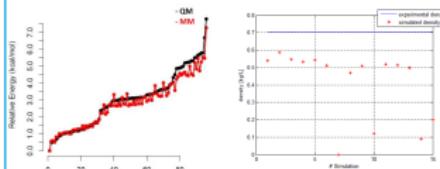


Figure 2: Fitted conformational energies in **red** compared to the quantum chemically calculated target data in **black**

5 - Current Status

Currently, the existing workflows in GROW for optimizing parameters towards micro-scale and macro-scale properties are being merged. So far these workflows cannot influence each other (see diagram below).



After the merging of the workflow has finished, the next step is to implement a combined loss function. Currently, following **loss function F** is minimized:

$$F(x) = \sum_{i=1}^n w_i \left(\frac{f_i^{exp} - f_i^{sim}}{f_i^{exp}} \right)^2$$

Where x is a vector containing the parameters $p_i: x = (p_1, p_2, \dots, p_n)^T$. Denoted by "exp" is the target data, whereas "sim" marks the iteratively performed simulations with the parameter set x . The weighting factors w_i are used to fine-tune $F(x)$.

The **loss function** that will be implemented for the combined workflow is:

$$F(x) = \sum_{i=1}^n w_i \left[\left(\frac{f_i^{exp,QM} - f_i^{sim,QM}(x)}{f_i^{exp,QM}} \right)^2 + \Omega_i w_i \left(\frac{f_i^{exp,MM} - f_i^{sim,MM}(x)}{f_i^{exp,MM}} \right)^2 \right]$$

The additional "QM" and "MM" are indicating that there are different types of target data and simulations. Denoted by "QM" are quantum mechanical calculations and simulations used for fitting the internal conformations energies, whereas "MM" marks the molecular mechanics components used to fit the density.

6 - Contact

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References:

- [1] "Relative electronic and free energies of octane's unimolecular conformations", Karl N. Kirschner, Wolfgang Heiden, Dirk Reith, DOI: 10.1080/00268976.2016.1262076.
- [2] "GROW: A gradient-based optimization workflow for the automated development of molecular models", Marco Hülsmann, Thorsten Küddermann, Jadran Vrabec, Dirk Reith DOI: <https://doi.org/10.1016/j.cpc.2009.10.024>



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Bonn-Rhein-Sieg
University of Applied Sciences

Optimization of force field parameters for molecular simulations

Lack of Affiliation Close to Title

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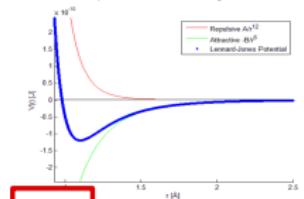
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No Research Question or Hypotheses

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The Lennard-Jones parameters σ and ϵ must be chosen such that the simulation results agree with target data. The target data consists of experimentally determined **bulk-phase density** (i.e. a macro-scale property) and **internal conformational energies** [1] (i.e. a micro-scale property) that are obtained using quantum chemistry calculations.

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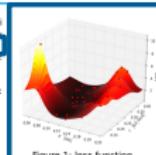


Figure 1: loss function

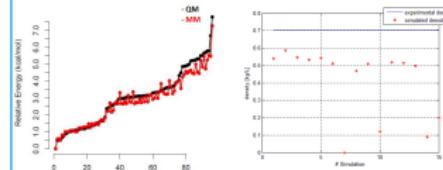
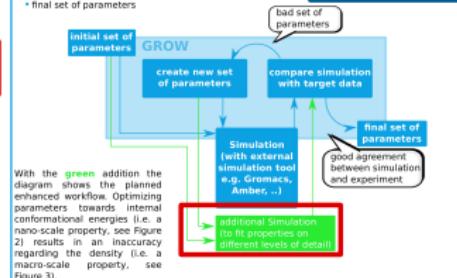


Figure 3: While the conformational energies fit quite well, the density derived from these simulations differ a lot from experimental determined

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The **loss function** that will be implemented for the combined workflow is:

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The additional "QM" and "MM" are indicating that there are different types of target data and simulations. Denoted by "QM" are quantum mechanical data and simulations used for fitting the internal conformations energies, whereas "MM" marks the molecular mechanic components used for the density.

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How the V-model can increase the efficiency of a research workflow

Background

The more the complexity of a scientific research or an engineering project increases, the more important becomes a structured workflow. According to [1] an inefficient way of working can consume at least 50 percent of the project effort and in the worst cases even 50 to 80 percent. Regarding this number, the poster presents a project management methodology called the V-Model, which was first proposed by Paul Rock [1]. In contrast to other research methodologies the V-shape of the model illustrates, that the testing phase can and should start at the very beginning of the project, to decrease the risk of a possible project failure at an early stage.

1 Talk/Read

After a possible topic of interest or an idea for an engineering project is narrowed, one of the first and most important steps is to search for suitable literature and the state of the art. It is necessary to define what a possible result of the project could be and what involved personalities like supervisor, customer, and other stakeholders expect in detail. The pie chart referring to [2], illustrates the importance of this step.



Validation (preferred legacy)

2 Requirements

Requirements serve the purpose of documenting the expectations of the supervisor or customer. While non-functional requirements describe the general conditions of the project like the given time frame or the budget, functional requirements describe the behavior of the developed product or software at a specific instant of time and scenario. The following graphic displays how requirements should be expressed referring to [3]:



Verification (preferred regular)

3 Development/ Research

One of the main advantages of the V-model is the allocation of different domain experts. By defining domains and defining interfaces between different modules or units of the project, this approach helps to isolate time consuming tasks from others, without affecting the whole project time frame. [4]



Conclusion

This poster demonstrates the importance of the inclusion of project stakeholders and the necessity of detailed project outcomes and requirements. The presented methodology divides complex systems into domain specific units that can be tested separately. The main advantage is given by the V-shape of the model, which offers the opportunity to perform verification and validation-loops on a regular basis. This process helps to identify possible failures and problems at an early stage, to intervene precociously and decrease the risk of wasting time and budget.

References

- [1] S. Muthu, A. Mulla, "Advancements in the V-Model", International Journal of Computer Applications, Vol. 100, 2014.
- [2] L. C. Rock, "Requirements Engineering", Arupdruck Gießen Heidelberg, 2000.
- [3] M. Gruska, "Towards the Automatic Generation of Software Test Cases from Requirements", IEEE Computer Society, 2003.
- [4] Vorleser Dozenten Informatik, Entwicklungsgesetz für mechanische Systeme, VDE 2000, Beuth Verlag GmbH, Düsseldorf, 2004.

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condition?
What
should
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Will
the system
offer the
possibility
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process
the
information

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5 Validation/ Documentation

The validation phase is necessary to check whether the developed project findings meet the expectations of the customer, moreover state-of-the-art. In contrast to the verification, the validation focuses on the expected result of the project and not on the requirements, as described in the following example.



4 Testing

This phase underlines the importance of the V-shape. Every module or unit of a domain can be tested separately against the requirements in a verification loop, which can be performed in parallel during the testing phase. Only if a unit has been tested successfully, the level of abstraction can be decreased to detect and eliminate possible failures at an early stage.

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This poster demonstrates the importance of the inclusion of project stakeholders and the necessity of detailed project outcomes and requirements. The presented methodology divides complex systems into domain specific units that can be quantified easily. The main advantage is given by the V-shape of the model, which provides the opportunity to perform verification- and validation-loops on a regular basis. This process helps to identify possible failures and problems at an early stage, to intervene precociously and decrease the risk of wasting time and budget.

References

- [1] S. Muthu, A. Mehta, "Advancements in the V-Model", International Journal of Computer Applications, Vol. 100, No. 10, 2014.
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- [4] Verena Dörmann (ed.), Projektmanagement für technologische Systeme, VDE 2009, Berlin/Vogel Verlag, Düsseldorf, 2009

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Additional references

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