Organização: Pró-Reitoria de Pesquisa - USP

Workshop de Capacitação em Escrita Científica

Módulo 1

Prof. Dr. Valtencir Zucolotto

Laboratório de Nanomedicina e Nanotoxicologia

Instituto de Física de São Carlos, USP

USP, 2012

Workshop Outline

Modulo 1: O Gênero Literário

Seções de Um Artigo Científico

Módulo 2: Estrutura 1: *Abstract*

Módulo 3: Estrutura 2: *Introduction*

Módulo 4: Estrutura 3: *Results and Discussion, Conclusion*

Módulo 5: Estilo

Linguagem 1: Especificidade, Complexidade e Ambiguidade

Módulo 6: Linguagem 2: Redundâncias, Ação no Verbo, Fluidez de Texto, Ritmo de Escrita

Módulo 7: Linguagem 3: *Plain English*, Escrever em Inglês, Preposições

Módulo 8: Linguagem 4: *Topic Sentences, Cover Letters*, *Final Remarks*

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Módulo 1

O Gênero Literário

Estrutura 1

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Why?, What?, When?....

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Why to Publish??

Publication is one of the most important steps of the scientist's work

If nobody knows, or can benefit from your work,

Why being at work ??

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

What do we Publish?

Scientists Publish Ideas !!

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

When to Publish?

When the initial

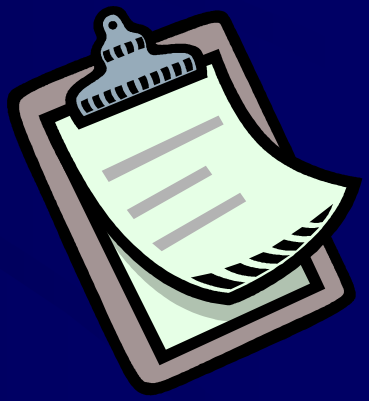
question/problem/hypothesis

had been answered/solved/tested !!!!!!

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

When to Publish?

Scientific Method / Hypothesis testing



Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

When to Publish?

-Distinct time scales for distinct areas;

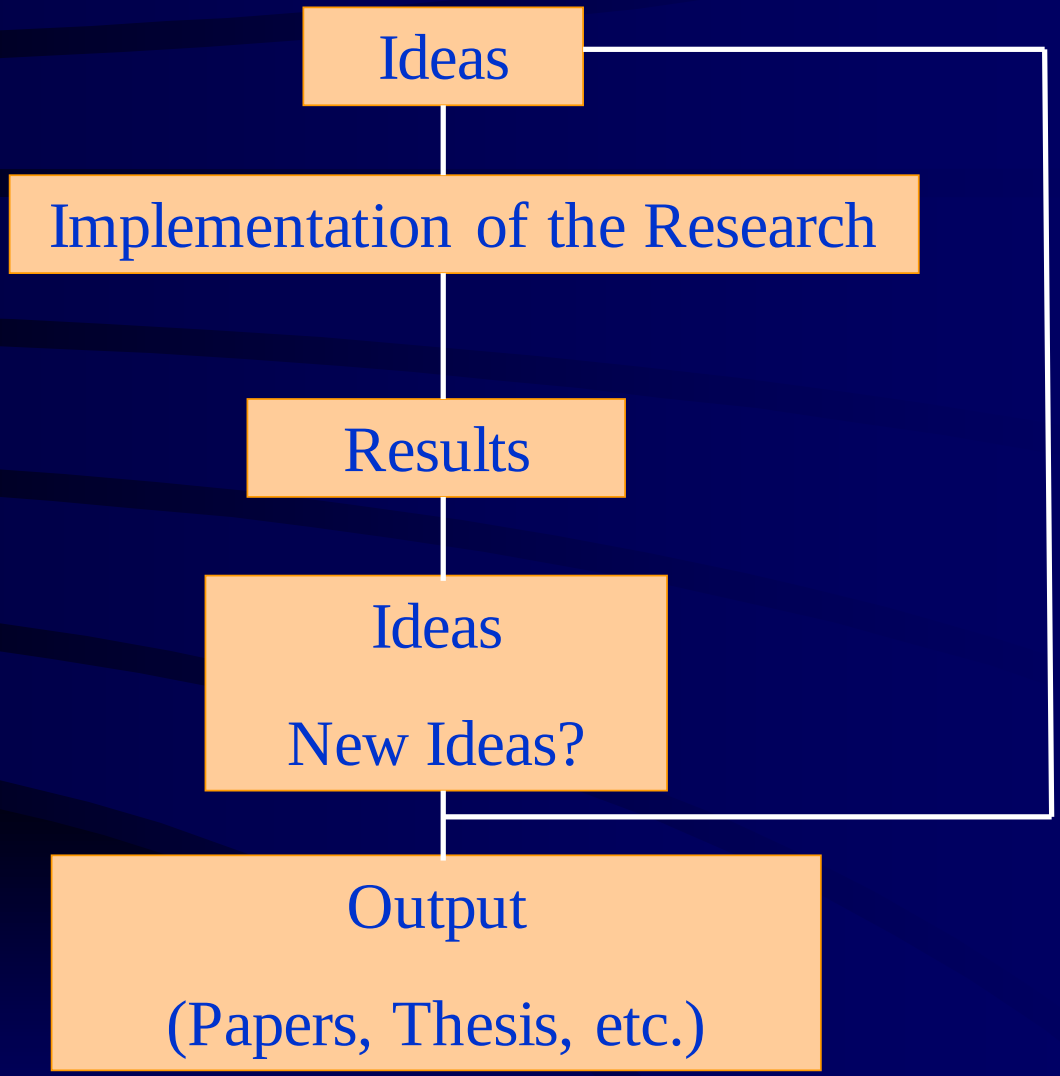
-Depends on the type of research:

Breakthroughs and Innovative research.

Advances on a specific, systematic investigation area.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Publishing Ideas



Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

1.
General Considerations

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Lesson Zero

Scientific writing as a “new” Literary Genre

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

A bit of History…

In the very beginning….

- Informal Letters exchanged by scientists.

- 1665: Creation of the first scientific periodical: *The Philosophical Transactions of the Royal Society*.

This new arena for discussion led to the development of a new genre:

The Scientific Report

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Audience

Who will read your paper?

Highly technical journal vs. less specific ones.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Clarity and Concision

Report your results clearly

Use as few words as necessary

Save words!!

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

References

All information or ideas must be referenced!

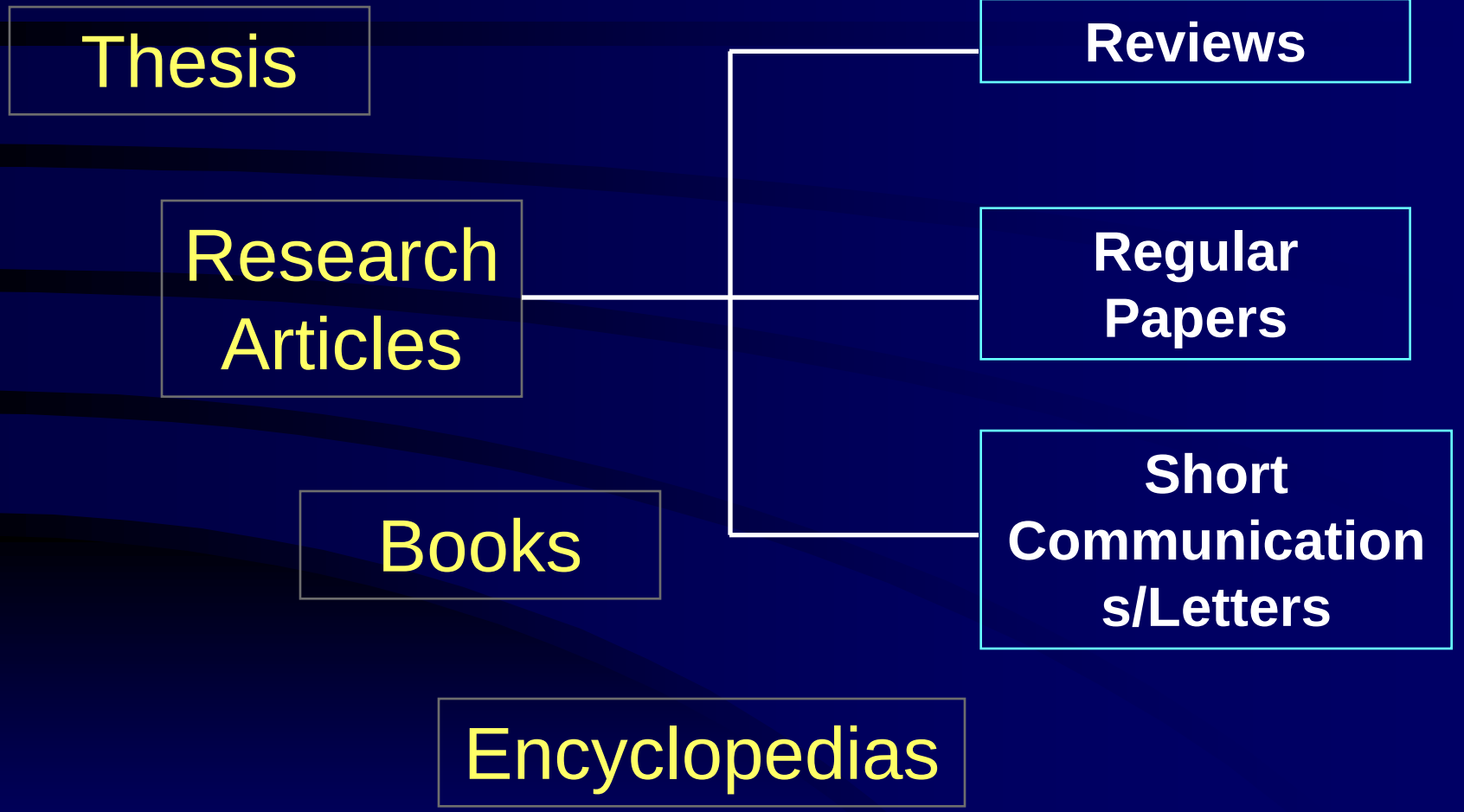
Including your own work

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

2.
Sections of a Regular Paper

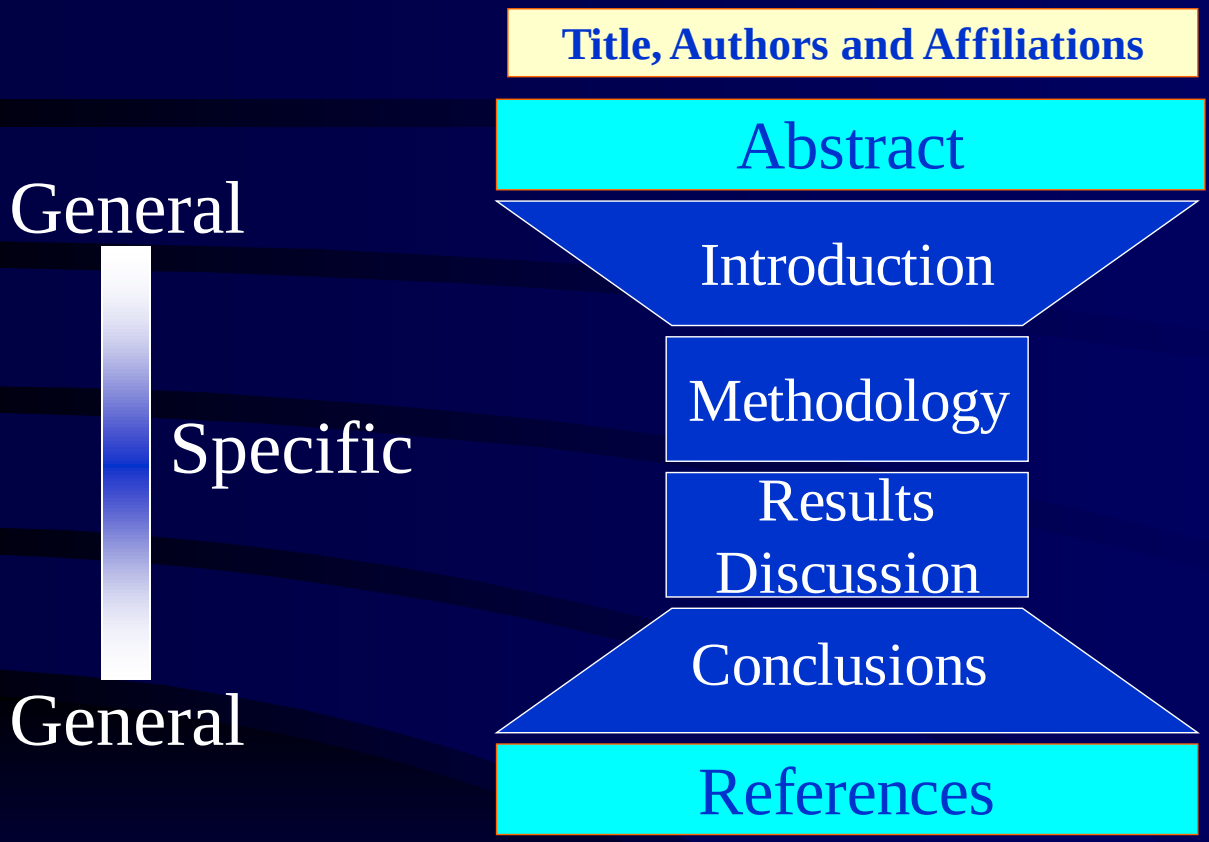
Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Types of Scientific Publications



Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Organization of a paper



Adapted from: Hill et al., Teaching ESL students to read and write experimental papers, TESOL Quarterly, 16: 333, 1982:

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Title, Authors and Affiliations

A good Title describes the contents of the paper

Function: to attract reader's attention

Use specific words strongly associated with the outcome of the paper: Keywords

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Title, Authors and Affiliations

Example 1: A paper reporting on the influence of the molecular weight on the mechanical properties of Polyaniline thin films:

Title 1: Mechanical properties of Polyaniline films

Poor, too general!

Title, Authors and Affiliations

Title 2: The influence of the MW on the Mechanical properties of polyaniline spin-coated films

Expresses the main idea of the work, the kind of film and its fabrication technique.

Keywords Included: mechanical properties, polyaniline, spin coated

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Title, Authors and Affiliations

Emphasize your key findings whenever possible

Title:

Metal-Polymer nanocomplexes induce spontaneous regression of lung tumors

OK!! The author describes the most important result shortly and concisely

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Title, Authors and Affiliations

Who are the authors of a paper?

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Title, Authors and Affiliations

Guidelines to define authorship:

All authors must be able to present/discuss/defend the paper.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Title, Authors and Affiliations

Authors Names Sequence:

First Name

The researcher who did the work, junior researcher.

Middle names

Anyone who intellectually contributed to the work

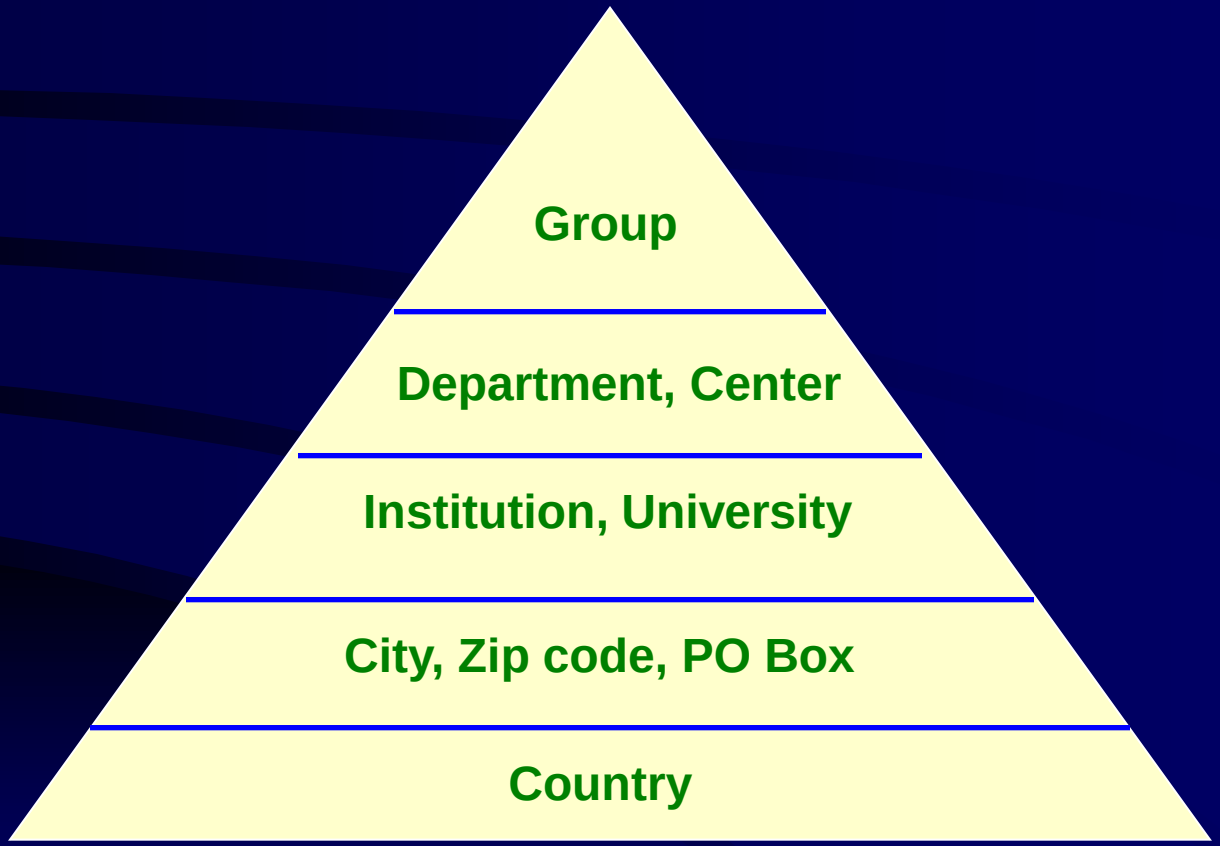
Last Name

The responsible for the research: supervisor/ group head/ senior scientist

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Title, Authors and Affiliations

Affiliations usually include the following information:



Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

A Model

Contextualization

Gap

Purpose

Methodology

Results

Conclusions

Aluísio, S.M. (1995). *Ferramentas para Auxiliar a Escrita de Artigos Científicos em Inglês como Língua Estrangeira*. **Tese de Doutorado**, IFSC-USP, 228 p.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Self-assembly of components larger than molecules into ordered arrays is an efficient way of preparing microstructured materials with interesting mechanical and optical properties. Although crystallization of identical particles or particles of different sizes or shapes can be readily achieved, the repertoire of methods to assemble binary lattices of particles of the same sizes but with different properties is very limited. This paper describes electrostatic self-assembly of two types of macroscopic components of identical dimensions using interactions that are generated by contact electrification. The systems we have examined comprise two kinds of objects (usually spheres) made of different polymeric materials that charge with opposite electrical polarities when agitated on flat, metallic surfaces. The interplay of repulsive interactions between like-charged objects and attractive interactions between unlike-charged ones results in the self-assembly of these objects into highly ordered, closed arrays. Remarkably, some of the assemblies that form are not electroneutral—that is, they possess a net charge. We suggest that the stability of these unusual structures can be explained by accounting for the interactions between electric dipoles that the particles in the aggregates induce in their neighbors.

Grzybowski et al., Nature Materials 2, 241–245 (2003)

Abstract

1) Context: Self-assembly of components larger than molecules into ordered arrays is an efficient way of preparing microstructured materials with interesting mechanical and optical properties.

2) GAP: Although crystallization of identical particles or particles of different sizes or shapes can be readily achieved, the repertoire of methods to assemble binary lattices of particles of the same sizes but with different properties is very limited.

3) Purpose: This paper describes electrostatic self-assembly of two types of macroscopic components of identical dimensions using interactions that are generated by contact electrification.

4) Methodology: The systems we have examined comprise two kinds of objects (usually spheres) made of different polymeric materials that charge with opposite electrical polarities when agitated on flat, metallic surfaces.

5) Results: The interplay of repulsive interactions between like-charged objects and attractive interactions between unlike-charged ones results in the self-assembly of these objects into highly ordered, closed arrays. Remarkably, some of the assemblies that form are not electroneutral—that is, they possess a net charge.

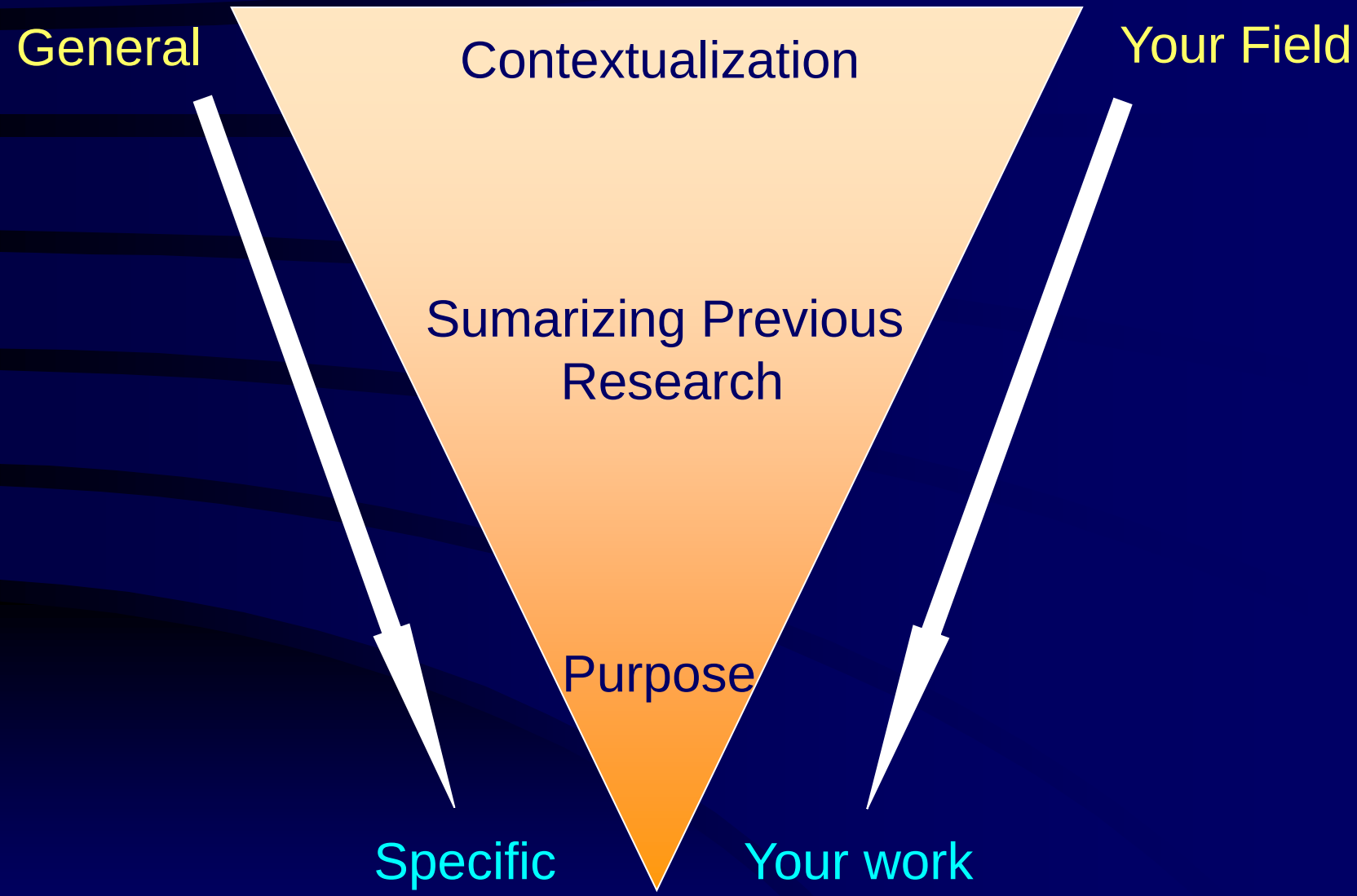
6) Conclusions: We suggest that the stability of these unusual structures can be explained by accounting for the interactions between electric dipoles that the particles in the aggregates induce in their neighbors.

Grzybowski et al., Nature Materials 2, 241–245 (2003)

Introduction

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Introduction



Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Methodology

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Methodology

Materials

What materials were employed?

Where did the materials come from?

Methods/Procedures

Reference to any well established methods and analyses

Details concerning the procedure adopted

Justifying the procedures adopted

Equipment

Equipment employed

Data analyses

Methods used for data processing and analyses

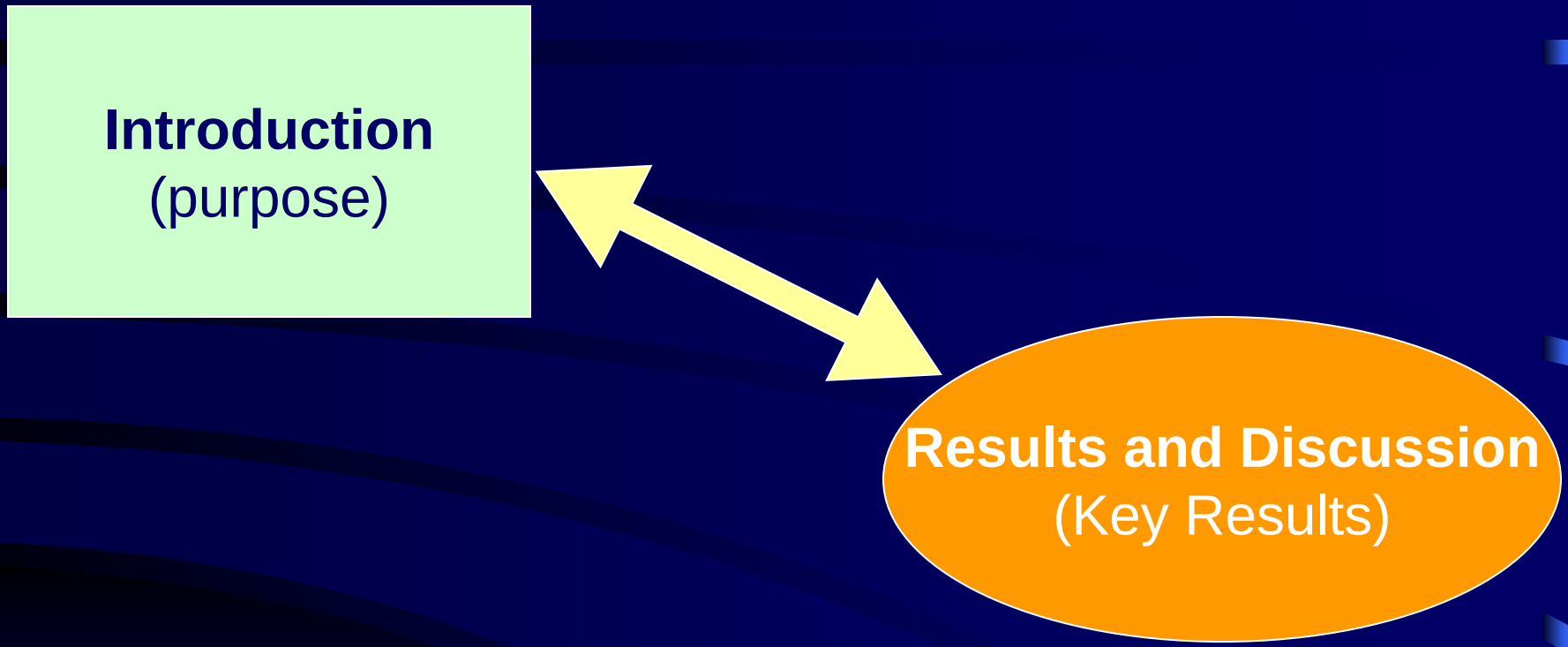
Prof. Dr. Valtencir Zucolotto

zuco@ifsc.usp.br

Results and Discussion

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Results



Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Conclusion

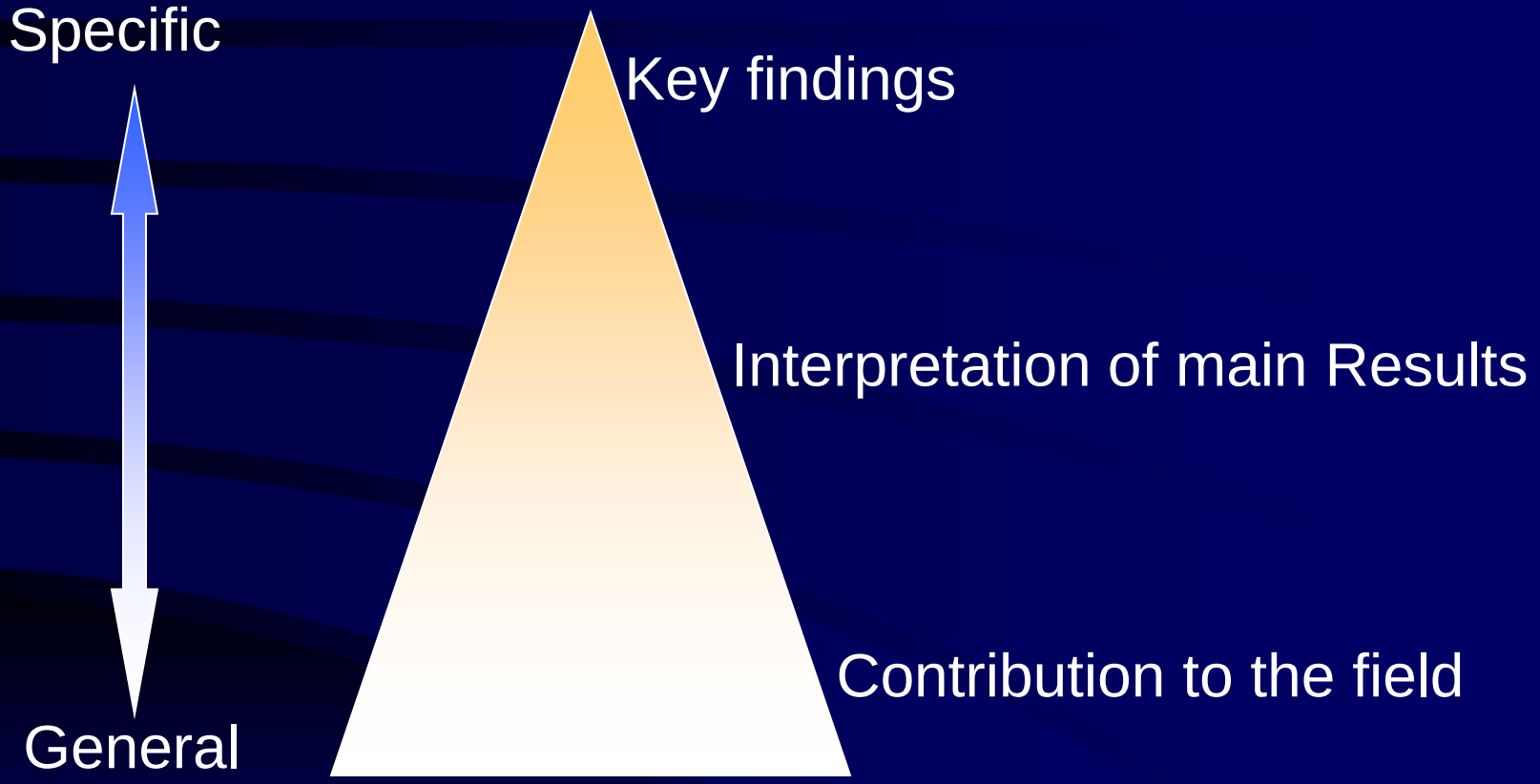
Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Conclusion

In contrast to the Introduction, the conclusions section starts the Specific–to–General Movement.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Conclusion



Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

References

All information or ideas must be referenced!

Including your own work

There are a number of different formats/styles you may use to cite other's work in the text, or arrange the references list:

Always consult the Journal's Guide for Authors

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

References

1. The citation-sequence system

References are numbered in the order they appear in the text.

Examples

"….However, recent reports have been made on the fabrication of ultrathin films of metallic phthalocyanines and polyelectrolytes via the electrostatic layer-by-layer technique (LBL).[10]

(10) Lutt, M.; Fitzsimmons, M. R.; Li, D. Q. *J. Phys. Chem. B* **1998**, *102*, 400.

References

2. The name-year system

References are listed alphabetically, using the first author´s last name.

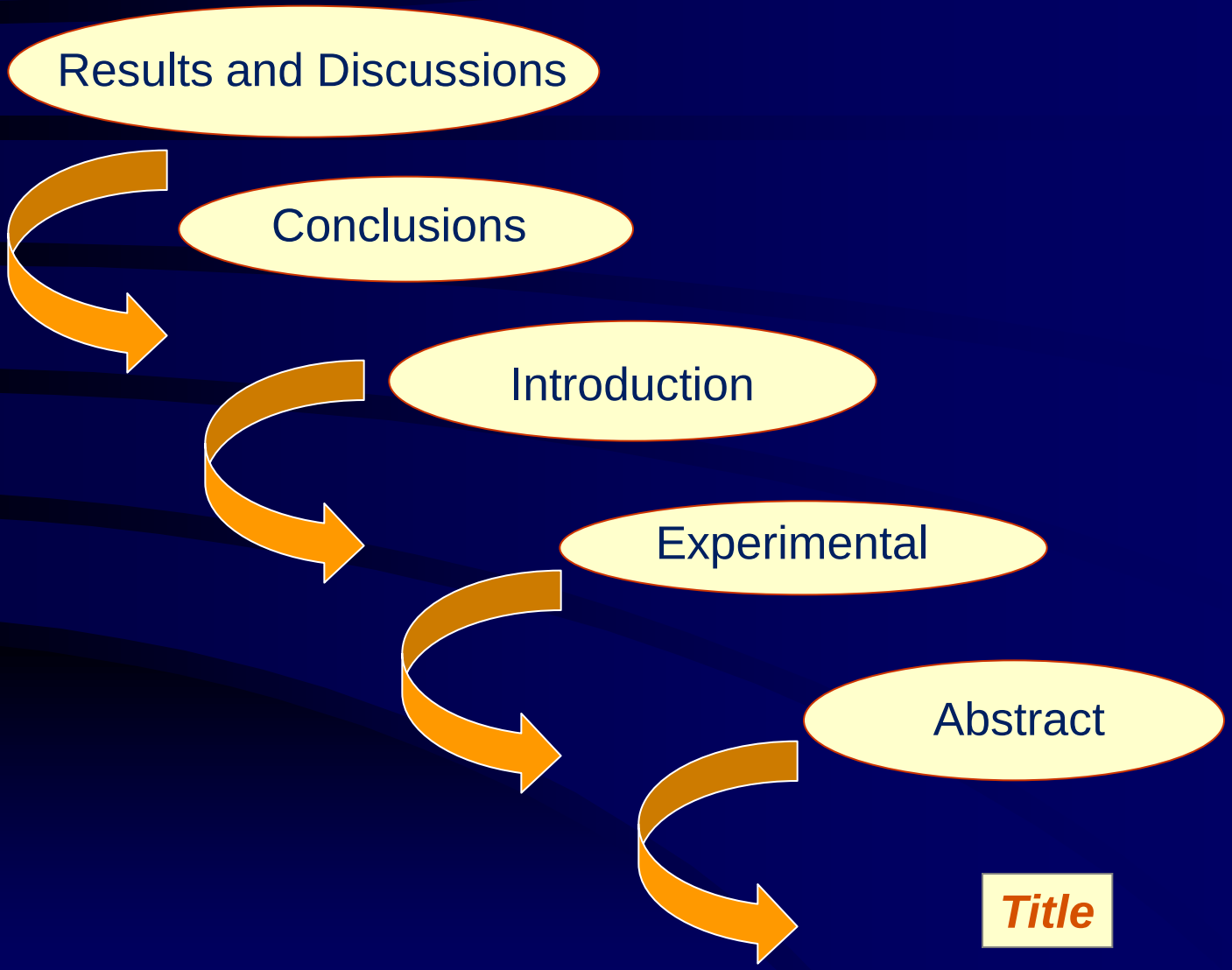
Examples

"….The layer-by-layer (LbL) technique has been largely employed in the immobilization of proteins and other biomolecules following the pioneering work of Lvov et al. [Lvov et al., 1993; Lvov et al., 1995]…."

Lvov, Y., Ariga, K., Ichinose, I., Kunitake, T., 1995. Assembly of multicomponent protein films by means of electrostatic layer-by-layer adsorption. J. Am. Chem. Soc.117, 6117- 6123.

Lvov, Y., Decher, G., Sukhorukov, G. 1993. Assembly of Thin Films by Means of Successive Deposition of Alternate Layers of DNA andv Poly(allylamine). Macromolecules 26, 5396-5399.

A Suggested Sequence….



Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Translations ??

Begin writing in English

Take your notes in English

Final version of a paper translated into English

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Plagiarism

You may cite others' words, data, etc. using your own words;

Do not paraphrase other author´s text

Do not paraphrase your early papers.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Plagiarism

As más condutas graves mais típicas e frequentes são as seguintes.

(a) A *fabricação*, ou afirmação de que foram obtidos ou conduzidos dados, procedimentos ou resultados que realmente não o foram.

(b) A *falsificação*, ou apresentação de dados, procedimentos ou resultados de pesquisa de maneira relevantemente modificada, imprecisa ou incompleta, a ponto de poder interferir na avaliação do peso científico que realmente conferem às conclusões que deles se extraem.

(c) O *plágio*, ou a utilização de ideias ou formulações verbais, orais ou escritas de outrem sem dar-lhe por elas, expressa e claramente, o devido crédito, de modo a gerar razoavelmente a percepção de que sejam ideias ou formulações de autoria própria.

http://www.fapesp.br/boaspraticas/codigo_fapesp0911.pdf

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Plagiarism

Relatório da Comissão de Integridade de Pesquisa do CNPq

A comissão instituída pela portaria PO-085/2011 de 5 de maio de 2011, constituída pelos pesquisadores Alaor Silvério Chaves, Gilberto Cardoso Alves Velho, Jaílson Bittencourt de Andrade, Walter Colli e coordenada pelo Dr. Paulo Sérgio Lacerda Beirão, diretor de Ciências Agrárias, Biológicas e da Saúde do CNPq, vem apresentar seu relatório final

Plágio: consiste na apresentação, como se fosse de sua autoria, de resultados ou conclusões anteriormente obtidos por outro autor, bem como de textos integrais ou de parte substancial de textos alheios sem os cuidados detalhados nas Diretrizes. Comete igualmente plágio quem se utiliza de ideias ou dados obtidos em análises de projetos ou manuscritos não publicados aos quais teve acesso como consultor, revisor, editor, ou assemelhado.

Autoplágio: consiste na apresentação total ou parcial de textos já publicados pelo mesmo autor, sem as devidas referências aos trabalhos anteriores.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Sources

-Introduction to Journal-Style Scientific Writing:

http://abacus.bates.edu/~ganderso/biology/resources/writing/HTWgeneral.html

-http://www.inter-biotec.com/biowc/style.html

-Scientific Writing, Easy When ou Know How, Peat, J., Elliot, E., Baur, L., Keena, V., BMJ Books, 2009

-Hill et al., Teaching ESL students to read and write experimental papers, TESOL Quarterly, 16: 333, 1982:

-Int. Committee of Medical J. Editors, Ann. Intern. Med., 1997, 126, 36.

Prof. Dr. Valtencir Zucolotto

zuco@ifsc.usp.br

Muito Obrigado

Valtencir Zucolotto

zuco@ifsc.usp.br

www.nanomedicina.com.br
www.lnn.ifsc.usp.br

www.twitter.com/Nanomedicina

Instituto de Física de São Carlos - USP

www.twitter.com/escreverartigos
www.twitter.com/writingpapers

Workshop de Capacitação em Escrita Científica

Módulo 2

Prof. Dr. Valtencir Zucolotto

Laboratório de Nanomedicina e Nanotoxicologia

Instituto de Física de São Carlos, USP

USP, 2012

Workshop Outline

Modulo 1: O Gênero Literário

Seções de Um Artigo Científico

Módulo 2: Estrutura 1: *Abstract*

Módulo 3: Estrutura 2: *Introduction*

Módulo 4: Estrutura 3: *Results and Discussion, Conclusion*

Módulo 5: Estilo

Linguagem 1: Especificidade, Complexidade e Ambiguidade

Módulo 6: Linguagem 2: Redundâncias, Ação no Verbo, Fluidez de Texto, Ritmo de Escrita

Módulo 7: Linguagem 3: *Plain English*, Escrever em Inglês, Preposições

Módulo 8: Linguagem 4: *Topic Sentences, Cover Letters*, *Final Remarks*

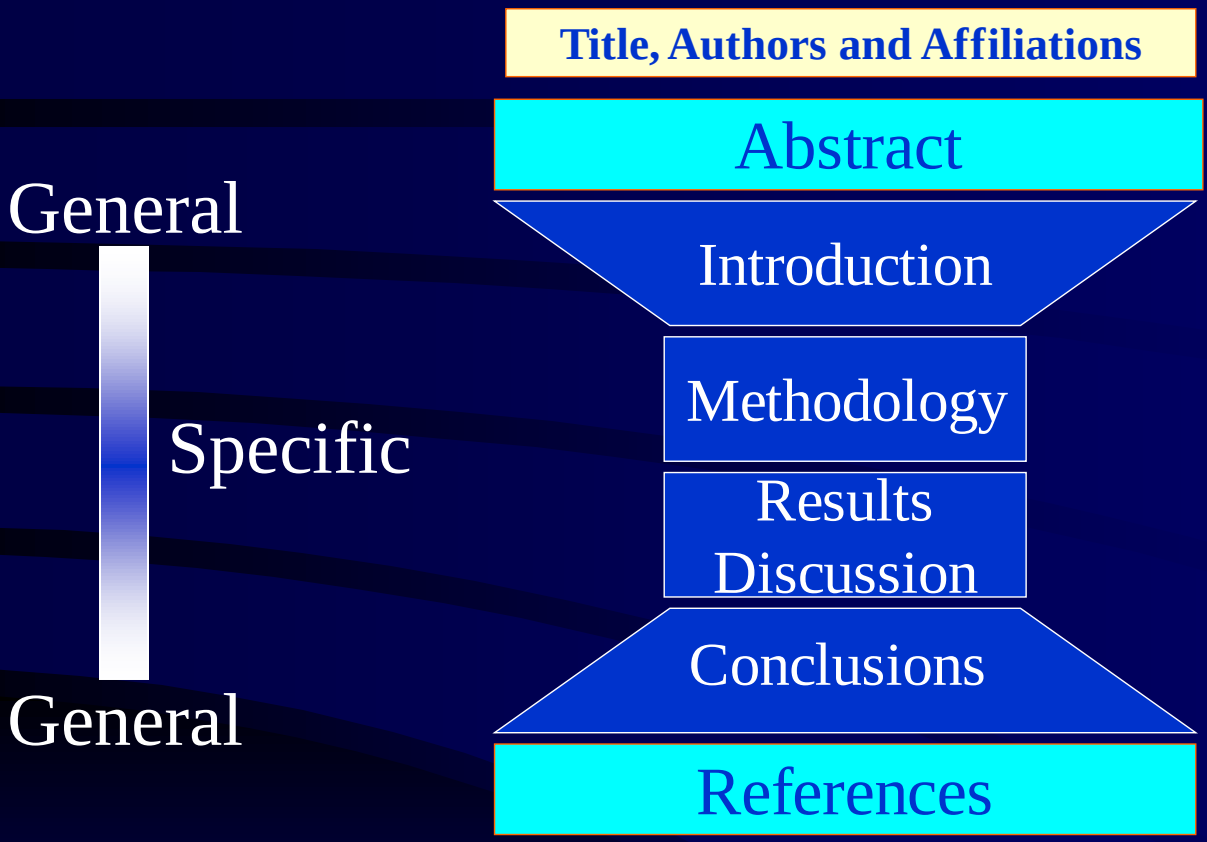
Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Módulo 2

Estrutura 1: Abstract

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Organization of a paper



Adapted from: Hill et al., Teaching ESL students to read and write experimental papers, TESOL Quarterly, 16: 333, 1982:

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

An abstract summarizes the major aspects of the paper

The abstract contains only text

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Informative	X	Descriptive
Contains all the relevant information of the paper		Describes only the nature/purpose of the study

Michael Alley *The Craft of Scientific Writing*, 3rd edition (Springer-Verlag, 1996).

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Style

- Past Tense (whenever possible);

- Active voice preferred;

- Concise, complete sentences.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Contextualization

Gap

Purpose

Methodology

Results

Conclusions

Aluísio, S.M. (1995). *Ferramentas para Auxiliar a Escrita de Artigos Científicos em Inglês como Língua Estrangeira*. **Tese de Doutorado**, IFSC-USP, 228 p.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

J Pharm Pharmaceut Sci 8(2):162-178, 2005

Abstract **PURPOSE**: Micellar solubilization is a powerful alternative for dissolving hydrophobic drugs in aqueous environments. In this work, we provide an insight into this subject. **METHODS**: A concise review of surfactants and micelles applications in pharmacy was carried out. **RESULTS**: Initially, a description of surfactants and aqueous micellar systems is presented. Following, an extensive review on micellar drug solubilization, including both the principles involved on this phenomenon and the work already done regarding solubilization of drugs by micelles is presented. The application of micelles in drug delivery, in order to minimize drug degradation and loss, to prevent harmful side effects, and to increase drug bioavailability, is also presented. Special emphasis is given to the more recent use of polymeric micelles. Finally, we briefly discuss the importance of surfactants and micelles as biological systems models as well as its application in micellar catalysis. **CONCLUSIONS**: As can be seen from the review presented, the use of micelles in pharmacy is an important tool that finds numerous applications.

Examples from the Literature

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Case 1

M2P1 Nature Mat

Self-assembly of components larger than molecules into ordered arrays is an efficient way of preparing microstructured materials with interesting mechanical and optical properties. Although crystallization of identical particles or particles of different sizes or shapes can be readily achieved, the repertoire of methods to assemble binary lattices of particles of the same sizes but with different properties is very limited. This paper describes electrostatic self-assembly of two types of macroscopic components of identical dimensions using interactions that are generated by contact electrification. The systems we have examined comprise two kinds of objects (usually spheres) made of different polymeric materials that charge with opposite electrical polarities when agitated on flat, metallic surfaces. The interplay of repulsive interactions between like-charged objects and attractive interactions between unlike-charged ones results in the self-assembly of these objects into highly ordered, closed arrays. Remarkably, some of the assemblies that form are not electroneutral—that is, they possess a net charge. We suggest that the stability of these unusual structures can be explained by accounting for the interactions between electric dipoles that the particles in the aggregates induce in their neighbors.

Grzybowski et al., Nature Materials 2, 241–245 (2003)

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

1) Context: Self-assembly of components larger than molecules into ordered arrays is an efficient way of preparing microstructured materials with interesting mechanical and optical properties.

2) GAP: Although crystallization of identical particles or particles of different sizes or shapes can be readily achieved, the repertoire of methods to assemble binary lattices of particles of the same sizes but with different properties is very limited.

3) Purpose: This paper describes electrostatic self-assembly of two types of macroscopic components of identical dimensions using interactions that are generated by contact electrification.

4) Methodology: The systems we have examined comprise two kinds of objects (usually spheres) made of different polymeric materials that charge with opposite electrical polarities when agitated on flat, metallic surfaces.

5) Results: The interplay of repulsive interactions between like-charged objects and attractive interactions between unlike-charged ones results in the self-assembly of these objects into highly ordered, closed arrays. Remarkably, some of the assemblies that form are not electroneutral—that is, they possess a net charge.

6) Discussion/Conclusions: We suggest that the stability of these unusual structures can be explained by accounting for the interactions between electric dipoles that the particles in the aggregates induce in their neighbors.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Case 2

M2P2 Nature Mat

Bioinert polyelectrolyte multilayers comprised of poly(acrylic acid) and polyacrylamide were deposited on colloidal particles (1.7 μm diameter) at low pH conditions by layer-by-layer assembly using hydrogen-bonding interactions. The multilayer films were coated uniformly on the colloidal particles without causing any flocculation of the colloids, and the deposited films were subsequently cross-linked by a single treatment of a carbodiimide aqueous solution. The lightly cross-linked multilayer films show excellent stability at physiological conditions (pH 7.4, phosphate-buffered saline), whereas untreated multilayer films dissolved. The multilayer-coated surfaces, both on flat substrates and on colloidal particles, exhibit excellent resistance toward mammalian cell adhesion. With this new solution-based cross-linking method, bioinert H-bonded multilayer coatings offer potential for biomedical applications.

Yang et al, **Langmuir**; 2004; 20; 5978

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Context??

Gap??

Purpose?: Bioinert polyelectrolyte multilayers comprised of poly(acrylic acid) and polyacrylamide were deposited on colloidal particles (1.7 μm diameter) at low pH conditions by layer-by-layer assembly using hydrogen-bonding interactions.

Methodology: The multilayer films were coated uniformly on the colloidal particles without causing any flocculation of the colloids, and the deposited films were subsequently cross-linked by a single treatment of a carbodiimide aqueous solution.

Results: The lightly cross-linked multilayer films show excellent stability at physiological conditions (pH 7.4, phosphate-buffered saline), whereas untreated multilayer films dissolved. The multilayer-coated surfaces, both on flat substrates and on colloidal particles, exhibit excellent resistance toward mammalian cell adhesion.

Conclusions: With this new solution-based cross-linking method, bioinert H-bonded multilayer coatings offer potential for biomedical applications.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Case 3

M2P3 Nature Biotech

Dendrimers are branched, synthetic polymers with layered architectures that show promise in several biomedical applications. By regulating dendrimer synthesis, it is possible to precisely manipulate both their molecular weight and chemical composition, thereby allowing predictable tuning of their biocompatibility and pharmacokinetics. Advances in our understanding of the role of molecular weight and architecture on the *in vivo* behavior of dendrimers, together with recent progress in the design of biodegradable chemistries, has enabled the application of these branched polymers as anti-viral drugs, tissue repair scaffolds, targeted carriers of chemotherapeutics and optical oxygen sensors. Before such products can reach the market, however, the field must not only address the cost of manufacture and quality control of pharmaceutical-grade materials, but also assess the long-term human and environmental health consequences of dendrimer exposure *in vivo*.

Lee *et al.*, **Nature Biotechnology 23**, 1517, 2005 ***(Review)***

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Abstract

Context: Dendrimers are branched, synthetic polymers with layered architectures that show promise in several biomedical applications. By regulating dendrimer synthesis, it is possible to precisely manipulate both their molecular weight and chemical composition, thereby allowing predictable tuning of their biocompatibility and pharmacokinetics. Advances in our understanding of the role of molecular weight and architecture on the *in vivo* behavior of dendrimers, together with recent progress in the design of biodegradable chemistries, has enabled the application of these branched polymers as anti-viral drugs, tissue repair scaffolds, targeted carriers of chemotherapeutics and optical oxygen sensors.

Gap: Before such products can reach the market, however, the field must not only address the cost of manufacture and quality control of pharmaceutical-grade materials, but also assess the long-term human and environmental health consequences of dendrimer exposure *in vivo*.

Descriptive or Informative ??

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 1

M2P4

Metallophthalocyanines (MPcs) are conjugated macrocyclic compounds that have been widely investigated in different scientific and technological fields. However, one of the limitations of the use of MPcs in technological devices is the limited solubility of these molecules, which makes difficult the deposition as thin films. This paper describes the use of the layer-by-layer technique to obtain thin films of cobalt tetrasulfonated phthalocyanine (CoTsPc) and the polyelectrolytes poly(allylamine hydrochloride) (PAH) and poly(amido amine) generation 4 (PAMAM G4). In addition to the structural investigations that revealed the nanoscale organization of the films, the possibility of using these platforms as humidity sensors has also been exploredA comprehensive SPR investigation on film growth reproduced dynamically the deposition process and provided an estimation of the layers' thicknesses. The electrical conductivity of the films deposited on interdigitated electrodes was found to be very sensitive to water vapor. This sensitivity is caused by the positioning of the Pc rings along the multilayers, which is a consequence of the self-assembly method. These results point to the development of a phthalocyanine-based humidity sensor obtained from a simple thin film deposition technique, whose outstanding ability to tailor molecular organization was crucial to achieve such high sensitivity.

Centurion et al., J. Nanosc. Nanotech, 2012 in press

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 2

M2P9 Nat Chem

Vibrational energy flow into reactants, and out of products, plays a key role in chemical reactivity, so understanding the microscopic detail of the pathways and rates associated with this phenomenon is of considerable interest. Here, we use molecular dynamics simulations to model the vibrational relaxation that occurs during the reaction CN1c-C6H12 HCN1 c-C6H11 in CH2Cl2, which produces vibrationally hot HCN. The calculations reproduce the observed energy distribution, and show that HCN relaxation follows multiple timescales. Initial rapid decay occurs through energy transfer to the cyclohexyl co-product within the solvent cage, and slower relaxation follows once the products diffuse apart. Re-analysis of the ultrafast experimental data also provides evidence for the dual timescales. These results, which represent a formal violation of conventional linear response theory, provide a detailed picture of the interplay between fluctuations in organic solvent structure and thermal solution-phase chemistry.

Glowacki et al., Nature Chem., 3, 850, 2011

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 3

M2P10 ACS Nano

Polymer nanoparticles are widely used as a highly generalizable tool to entrap a range of different drugs for controlled or site-specific release. However, despite numerous studies examining the kinetics of controlled release, the biological behavior of such nanoparticles remains poorly understood, particularly with respect to endocytosis and intracellular trafficking. We synthesized polyethyleniminedecorated polymer nanospheres (ca. 100 250 nm) of the type commonly used for drug release and used correlated electron microscopy, fluorescence spectroscopy and microscopy, and relaxometry to track endocytosis in neural cells. These capabilities provide insight into how polyethylenimine mediates the entry of nanoparticles into neural cells and show that polymer nanosphere uptake involves three distinct steps, namely, plasma membrane attachment, fluid-phase as well as clathrin- and caveolinindependent endocytosis, and progressive accumulation in membrane-bound intracellular vesicles. These findings provide detailed insight into how the intracellular delivery of nanoparticles is mediated by polyethylenimine, which is presently the most commonly used nonviral gene transfer agent. This fundamental knowledge may also assist in the preparation of next-generation nonviral vectors.

Evans et al., ACS Nano, In Press

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 4

Currently, mass spectrometry-based protein bioanalysis is primarily achieved through monitoring the representative peptide(s) resulting from analyte protein digestion. However, this approach is often incapable of differentiating the measurement of protein analyte from its post-translational modifications (PTMs) and/or potential biotransformation (BTX) products. This disadvantage can be overcome by direct measurement of the intact protein analytes. Selected reaction monitoring (SRM) on triple quadrupole mass spectrometers has been used for the direct measurement of intact protein. However, the fragmentation efficiency though the SRM process could be limited in many cases, especially for high molecular weight proteins. In this study, we present a new strategy of intact protein bioanalysis by high-resolution (HR) full scan mass spectrometry using human lysozyme as a model protein. An HR linear ion-trap/ Orbitrap mass spectrometer was used for detection. A composite of isotopic peaks from one or multiple charge states can be isolated from the background and used to improve the signal-to-noise ratio. The acquired data were processed by summing extracted ion chromatograms (EIC) of the 10 most intense isotopic ions of octuply protonated lysozyme. Quantitation of the plasma lysozyme was conducted by utilizing high resolving power and an EIC window fitting to the protein molecular weight. An assay with a linear dynamic range from 0.5 to 500 µg/mL was developed with good accuracy and precision. The assay was successfully employed for monitoring the level of endogenous lysozyme and a potential PTM in human plasma. The current instrumentation limitations and potential advantages of this approach for the bioanalysis of large proteins are discussed.

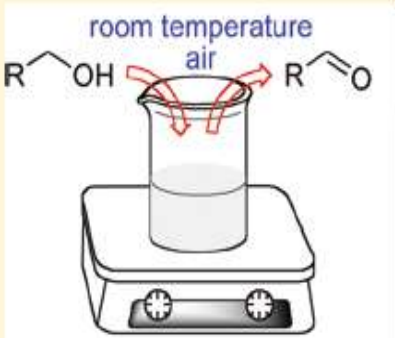
Juan et al., Analytical Chem, In Press

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

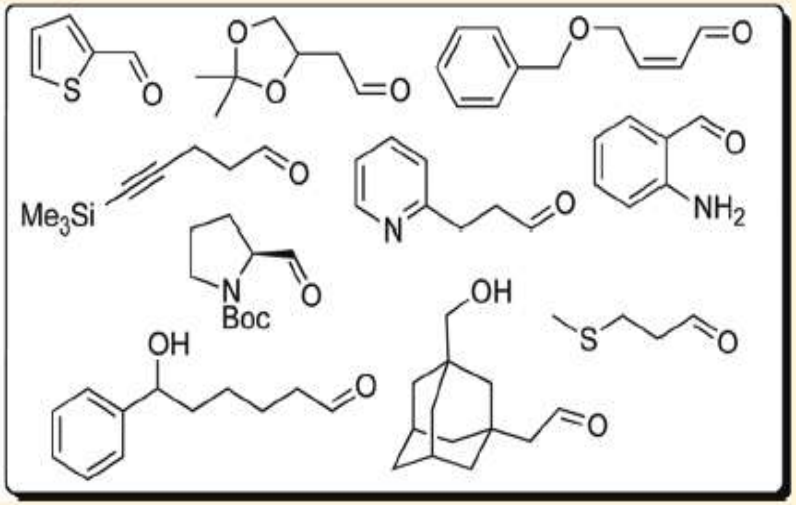
Prática 5

M2P12 JACS

ABSTRACT:



Catalyst:
5 mol % (bpy)Cu^{I}X
5 mol % TEMPO
10 mol % *N*-methylimidazole



Aerobic oxidation reactions have been the focus of considerable attention, but their use in mainstream organic chemistry has been constrained by limitations in their synthetic scope and by practical factors, such as the use of pure O_2 as the oxidant or complex catalyst synthesis. Here, we report a new (bpy)Cu^{I}/TEMPO catalyst system that enables efficient and selective aerobic oxidation of a broad range of primary alcohols, including allylic, benzylic, and aliphatic derivatives, to the corresponding aldehydes using readily available reagents, at room temperature with ambient air as the oxidant. The catalyst system is compatible with a wide range of functional groups and the high selectivity for 1° alcohols enables selective oxidation of diols that lack protecting groups.

Hoover et al., J. Am. Chem. Soc. 133, 16901, 2011

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 6

M2P5 IEEE Sig Proc

Accurate and low-cost sensor localization is a critical requirement for the deployment of wireless sensor networks in a wide variety of applications. Low-power wireless sensors may be many hops away from any other sensors with a priori location information. In cooperative localization, sensors work together in a peer-to-peer manner to make measurements and then form a map of the network. Various application requirements (such as scalability, energy efficiency, and accuracy) will influence the design of sensor localization systems. In this article, we describe measurement-based statistical models useful to describe time-of-arrival (TOA), angle-of-arrival (AOA), and received-signal-strength (RSS) measurements in wireless sensor networks. Wideband and ultra-wideband (UWB) measurements, and RF and acoustic media are also discussed. Using the models, we show how to calculate a Cramér-Rao bound (CRB) on the location estimation precision possible for a given set of measurements. This is a useful tool to help system designers and researchers select measurement technologies and evaluate localization algorithms. We also briefly survey a large and growing body of sensor localization algorithms. This article is intended to emphasize the basic statistical signal processing background necessary to understand the state-of-the-art and to make progress in the new and largely open areas of sensor network localization research.

IEEE Signal Processing Magazine, 2005, p 55

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 7

M2P6 Int J Plast

Commercial canmaking processes include drawing, redrawing and several ironing operations. It is experimentally observed that during the drawing and redrawing processes earing develops, but during the ironing processes earing is reduced. It is essential to understand the earing mechanism during drawing and ironing for an advanced material modeling. A new analytical approach that relates the earing profile to r-value and yield stress directionalities is presented in this work. The analytical formula is based on the exact integration of the logarithmic strain. The derivation is for a cylindrical cup under the plane stress condition based on rigid perfect plasticity while force equilibrium is not considered. The earing profile is obtained solely from anisotropic plastic properties in simple tension. The earing mechanism is explained from the present theory with explicit formulae. It has been proved that earing is the combination of the contributions from r-value and yield stress directionalities. From a directionality (y-axis) vs. angle from the rolling (x-axis) plot, the earing profile is generated to be a scaled mirror image of the r-value directionality with respect to 90 (x = 90) and also a scaled mirror image of the yield stress directionality with respect to the reference yield stress (y = 1). Three different materials (Al–5% Mg alloy, AA 2090-T3 and AA 3104 RPDT control coil) are considered for verification purposes. This approach provides a fundamental basis for understanding the earing mechanism. In practice, the present theory is also very useful for the prediction of the earing profile of a drawn and iron cup and its related convolute cut-edge design for an earless cup.

International Journal of Plasticity 27 (2011) 1165

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 8

M2P7 Int J electron

Network-on-chip (NoC) is considered the next generation of communication infrastructure, which will be omnipresent in different environments. In the platform-based design methodology, an application is implemented by a set of collaborating intellectual property (IP) blocks. The selection of the most suited set of IPs as well as their physical mapping onto the NoC to efficiently implement the application at hand are two hard combinatorial problems. In this article, we propose an innovative power-aware multi-objective evolutionary algorithm to perform the assignment and mapping stages of a platform-based NoC design synthesis tool. Our algorithm uses the well-known multi-objective evolutionary algorithms NSGA-II and microGA as kernels. The optimisation is driven by the required area and the imposed execution time, considering that the decision maker's restriction is the power consumption of the implementation.

International Journal of Electronics, 97, 2010, 1163

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 9

M2P13 IEEE T.E.C.

Design optimization problems in chemical engineering and in many other engineering domains are characterized by the presence of a large number of discrete and continuous decision variables, complex nonlinear models that restrict the search space, nonlinear cost functions, and the presence of many local optima. The classical approach to such problems are mixed integer nonlinear program solvers that work on a superstructure formulation which explicitly represents all design alternatives. The structural decisions lead to a large number of discrete variables and an exponential increase in the computational effort. The mathematical programming (MP) methods which are usually employed to solve the continuous subproblems that arise by fixing the discrete variables provide only one local optimum which depends strongly on the initialization. Thus standard methods may not find the global optimum despite long computation times. In this contribution we introduce a memetic algorithm (MA) for the global optimization of a computational demanding real-world design problem from the chemical engineering domain. The MA overcomes the problem of getting stuck in local optima by the use of an evolution strategy (ES) which addresses the global optimization of the design decisions, whereas a robust MP solver is used to handle complex nonlinear constraints as well as to improve the individuals of the ES by performing a local search in continuous sub-spaces in an integrated fashion. The MA is discussed in detail, the novel decomposition of the problem class at hand is analyzed and the MA is tested for the example of the optimal design of a reactive distillation column with several thousand decision variables. The MA is the only algorithm that finds the global solution in reasonable computation times. The introduction of structural decisions and additional constraints and discontinuous penalty terms lead only to a moderate increase in the computational effort which demonstrates the potential of this class of memetic algorithms in real-world design optimization problems.

Urselmann, et al., IEEE Transactions on Evolutionary Computation, 15, 2011, 659

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 10

M2P14 Int J Inf

The problem of predicting the next request during a user's navigation session has been extensively studied. In this context, higher-order Markov models have been widely used to model navigation sessions and to predict the next navigation step, while prediction accuracy has been mainly evaluated with the hit and miss score.We claim that this score, although useful, is not sufficient for evaluating next link prediction models with the aim of finding a sufficient order of the model, the size of a recommendation set, and assessing the impact of unexpected events on the prediction accuracy. Herein, we make use of a variable length Markov model to compare the usefulness of three alternatives to the hit and miss score: the Mean Absolute Error, the Ignorance Score, and the Brier score. We present an extensive evaluation of the methods on real data sets and a comprehensive comparison of the scoring methods.

Borges et al., International Journal of Information Technology & Decision Making, 9, 2010, 547.

Prática 11

M2P15 Human Comp Int

Educative sensemaking focuses on the needs of self-directed learners, a nonexpert population of thinkers who must locate relevant information sources, evaluate the applicability and accuracy of digital resources for learning, and determine how and when to use these resources to complete educational tasks. Self-directed learners face a sensemaking paradox: They must employ deep-level thinking skills to process information sources meaningfully, but they often lack the requisite domain knowledge needed to deeply analyze information sources and to successfully integrate incoming information with their own existing knowledge. In this article, we focus on the needs of college-aged students engaged in learning about natural sciences using web-based learning resources. We explored the impact of cognitive personalization technologies on students' sensemaking processes using a controlled study in which students' cognitive and metacognitive processes were analyzed as they completed a common educational task: writing an essay.We coded students' observable on-screen behaviors, selfreported processes, final essays, and responses to domain assessments to assess benefits of personalization technologies on students' educative sensemaking. Results show that personalization supported students' analysis of knowledge representations, helped students work with their representations in meaningful ways, and supported effective encoding of new knowledge. We discuss implications for new technologies to help students overcome the educative sensemaking paradox.

Butcher et al., Human–Computer Interaction, 26, 2011,123.

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Prática 12

Reordene as frases da maneira correta, categorizando-as:

M2P8 Nature Mat

Here we report that dentin matrix protein 1 (DMP1), an acidic protein, can nucleate the formation of hydroxyapatite in vitro in a multistep process that begins by DMP1 binding calcium ions and initiating mineral deposition.

Bones and teeth are biocomposites that require controlled mineral deposition during their self-assembly to form tissues with unique mechanical properties.

Acidic extracellular matrix proteins play a pivotal role during biomineral formation.

The nucleated amorphous calcium phosphate precipitates ripen and nanocrystals form. Subsequently, these expand and coalesce into microscale crystals elongated in the c-axis direction.

Protein-mediated initiation of nanocrystals, as discussed here, might provide a new methodology for constructing nanoscale composites by self-assembly of polypeptides with tailor-made peptide sequences.

However, the mechanisms of protein-mediated mineral initiation are far from understood.

Characterization of the functional domains in DMP1 demonstrated that intermolecular assembly of acidic clusters into a -sheet template was essential for the observed mineral nucleation.

Nature Materials 2, 552–558, 2003

Prof. Dr. Valtencir Zucolotto
zuco@ifsc.usp.br

Sources

Source: Michael Alley *The Craft of Scientific Writing*, 3rd edition (Springer-Verlag, 1996).

Hill et al., Teaching ESL students to read and write experimental papers, TESOL Quarterly, 16: 333, 1982:

Aluísio, S.M. (1995). *Ferramentas para Auxiliar a Escrita de Artigos Científicos em Inglês como Língua Estrangeira*. **Tese de Doutorado**, IFSC-USP, 228 p.

Grzybowski et al., Nature Materials 2, 241–245 (2003)

Yang et al, **Langmuir**; 2004; 20; 5978

Lee *et al.,* **Nature Biotechnology 23**, 1517, 2005 ***(Review)***

Centurion et al., J. Nanosc. Nanotech, 2011 in press

Glowacki et al., Nature Chem., 3, 850, 2011

IEEE Signal Processing Magazine, 2005, p 55

Borges et al., International Journal of Information Technology & Decision Making, 9, 2010, 547.

International Journal of Plasticity 27 (2011) 1165

Urselmann, et al., IEEE Transactions on Evolutionary Computation, 15, 2011, 659

Evans et al., ACS Nano, In Press

Juan et al., Analytical Chem, In Press

Butcher et al., Human–Computer Interaction, 26, 2011,123.

International Journal of Electronics, 97, 2010, 1163

Nature Materials 2, 552–558, 2003

Hoover et al., J. Am. Chem. Soc. 133, 16901, 2011

Prof. Dr. Valtencir Zucolotto

zuco@ifsc.usp.br

Muito Obrigado

Valtencir Zucolotto

zuco@ifsc.usp.br

www.nanomedicina.com.br

www.lnn.ifsc.usp.br

www.twitter.com/Nanomedicina

Instituto de Física de São Carlos - USP

www.twitter.com/escreverartigos

www.twitter.com/writingpapers