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2nd Basic and Clinical Immunogenomics
and
3rd Immunoinformatics (Immunomics) Conferences

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International Immunomics Society
Hungarian Academy of Sciences

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OBJECT ORIENTED IMPLEMENTATION OF A SIMULATION MODEL FOR T-CELL ACTIVATION

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The interaction between T-Cells (TCs) and antigen presenting Cells (APCs) is characterized by a large variety of different interaction partners, in particular within the TC (TCR, Lck, CD4, CD48, zap) and MHC within the APC. No computer model whatsoever can include all possible candidates, not to speak of adequately assigning physiological values to their parameters. When building a simulation software it's clear from the start that several (different) sets of partners (molecules) with correspondingly different interactions have to be modelled, evaluated and compared. This necessitates to add and withdraw molecules (objects) of different types with high flexibility. These requirements strongly call for an object oriented approach of implementation which we followed in the framework of Java.

Besides the Cell classes for the APC and the TC we implemented a base Molecules class (implementing some basic functions) and it's derived subclasses like the TCR and MHC class. Furthermore there are classes for parameter input, corresponding to the concept of Java's property files, and classes for molecule interaction.

The output in ASCII coded format is submitted to the Statistical Analysis System (SAS) for evaluation. The simulation parameters also are submitted to SAS in eXtendible Markup Language (XML) format. We also implemented a software management, a batch processing mode and the possibility of intermediate checkpoints to continue or rerun simulation jobs.

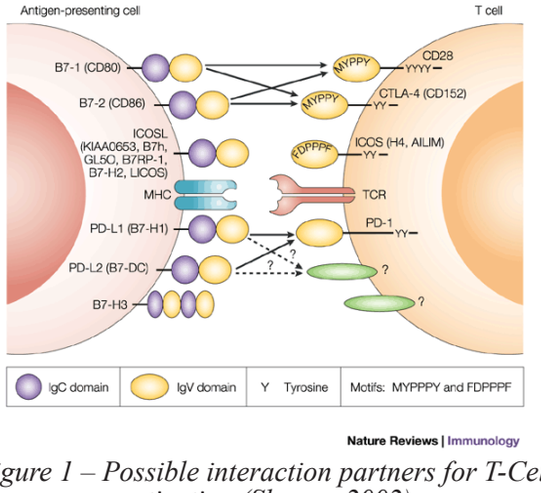

Figure 1 – Possible interaction partners for T-Cell activation (Sharpe, 2002)

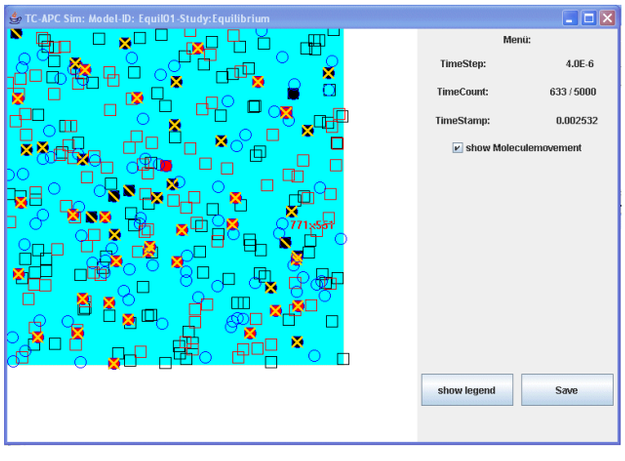

Figure 2 – A snapshot of the computer model simulating T-Cell activation

REFERENCES:

Sharpe AH, Freeman GJ. (2002), The B7-CD28 superfamily, Nat. Rev. Immunol., 2002; 2:116-26

Object Oriented Implementation Of T-Cell Activation

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Introduction

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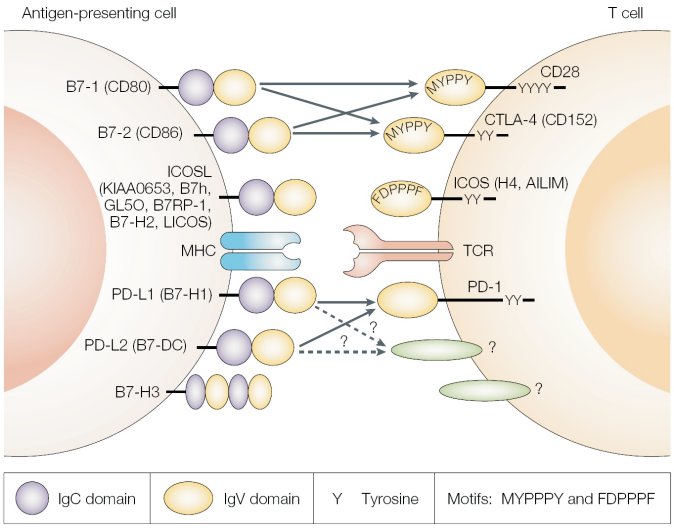

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Methods

No computer model whatsoever can include all possible candidates, not to speak of adequately assigning physiological values to their parameters. When building a simulation software it's clear from the start that several (different) sets of partners (molecules) with correspondingly different interactions have to be modelled, evaluated and compared. This necessitates to add and withdraw molecules (objects) of different types with high flexibility. These requirements strongly call for an object oriented approach of implementation which we followed in the framework of Java.

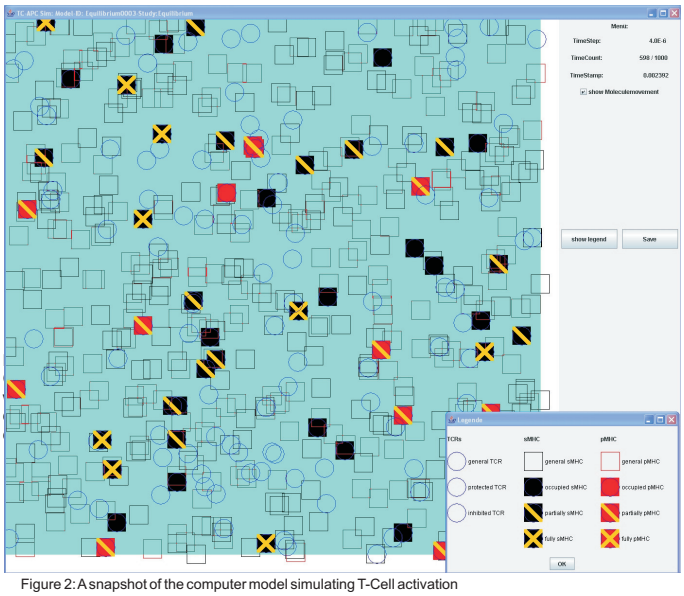

Figure 2: A snapshot of the computer model simulating T-Cell activation

Besides the cell classes for the APC and the TC we implemented a base class 'Molecule' (implementing some basic functions) and it's derived subclasses such as TCR and MHC class. Furthermore there are classes for parameter input, corresponding to the concept of Java's property files, and classes for molecule interaction.

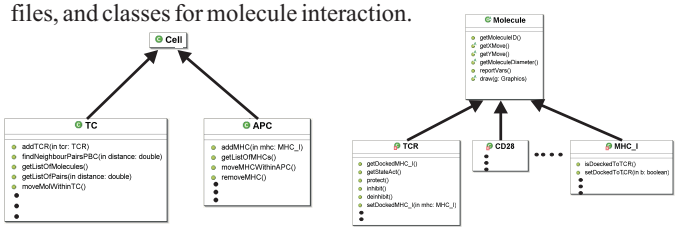

Figure 3: General functionalities and attributes of cells are defined in a parent (abstract) class 'Cell', wheras specific features can easily be added in derifed subclasses (APC, TC). Simularly, classes for specific molecules (TCR, MHC, CD28) are derifed from a more general, parent class 'Molecule'. Following the object oriented hierarchial design provides an optimum basis for coherent extension of software so as to include new types of molecules.

Software design in an interdisciplinary cooperation

Modeling and simulation of immune reactions has to cope with continously changing aspects of theory and experimental results.
Several paradigms are circulated within the scientific community, putting emphasis on different sets of 'most important' molecules.
Therefor we tried from the start to design the software as flexible as possible. Additionaly, we evaluated the use of 'design tools', such as Omondo . With their help, standardized diagrams in 'Unified Modeling Language' (UML) can be produced. On the one hand these diagrams can be readily discussed with immunologists, even if they are not familiar with software concepts. In particular, the decision trees within the model, representing the branching into different reaction pathways, proved extremly helpful.

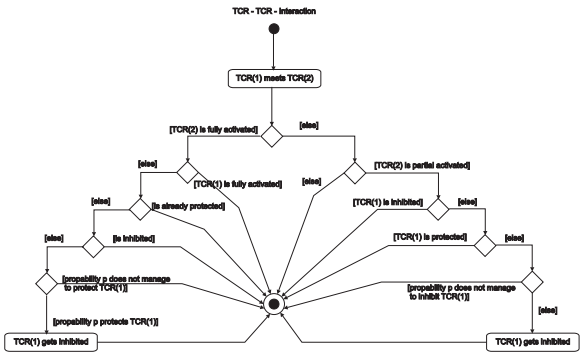

Figure 4: TCR-TCR interaction modeled as UML-diagram.

Acknowledgements

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