



publications

Listing in reversed chronological order.

Scientific Journals and Refereed Proceedings:

S. Pilari, L. Fronton and W. Huisinga

Monoclonal Antibody Disposition beyond Target Binding: Impact of FcRn on Clearance and Derivation of Mechanistic Compartment Models

Submitted (2011).

S. Menz, R. Matthiesen, C. Dehmel, C. Barembruch, R. Hengge and W. Huisinga.

Precise Switching of Flagellar Gene Expression in Escherichia Coli by the FlgM-FlhA Regulatory Network.

Preprint (2010).

S. Menz, J.C. Latorre, C. Schütte and W. Huisinga

Hybrid stochastic-deterministic solution of the chemical master equation

SIAM Multiscale Modelling and Simulation, 10 (2012) pp. 1232-1262

Journal (<http://epubs.siam.org/doi/abs/10.1137/110825716>)

W. Huisinga, A. Solms, L. Fronton and S. Pilari

Modeling inter-individual variability in physiologically-based pharmacokinetics and its link to mechanistic covariate modeling

CPT: Pharmacometrics & Systems Pharmacology, 1 (2012), e4.

Journal (<http://dx.doi.org/10.1038/psp.2012.3>) (open access), Suppl Material (Data (<http://www.nature.com/psp/journal/v1/n9/extref/psp20123x1.pdf>) & Matlab code (<http://www.nature.com/psp/journal/v1/n9/extref/psp20123x2.zip>))

B.-F. Krippendorff, D. A. Oyarzún and W. Huisinga

Predicting the F(ab)-mediated effect of monoclonal antibodies in vivo by combining cell-level



kinetic and pharmacokinetic modelling

J. Pharmacokinet. Pharmacodyn. 39 (2012), pp 125-139.

Journal (<http://www.springerlink.com/content/4u47pg2km665012t/fulltext.pdf>) (open access)

M. von Kleist, S. Menz, H. Stocker, K. Arasteh, C. Schütte, W. Huisinga

HIV Quasispecies Dynamics during Pro-Active Treatment Switching: Impact on Multi-Drug Resistance and Resistance Archiving in Latent Reservoirs

PLoS ONE, Vol. 6 (2011), e18204.

Journal (<http://dx.doi.org/10.1371/journal.pone.0018204>) (open access)

A. Y. Weiße, and W. Huisinga

Error-Controlled Global Sensitivity Analysis of Ordinary Differential Equations

J. Comput. Phys. 230 (2011), pp 6824-6842.

Journal (<http://dx.doi.org/10.1016/j.jcp.2011.05.011>)(open access), Suppl Material (zip (http://compphysiol.math.uni-potsdam.de/pub/WeisseHuisinga_JCP2011_GlobalSensitivityODE-Matlab-supplement.zip))

S. Pilari, C. Preusse and W. Huisinga

Gestational Influences on the Pharmacokinetics of Gestagenic Drugs: A Combined In Silico, In Vitro and In Vivo Analysis

Eur J Pharm Sci., 42 (2011), pp. 318-331.

Journal (<http://dx.doi.org/10.1016/j.ejps.2010.12.003>)

W. Huisinga and B.-F. Krippendorff

Eine gute Dosis Mathematik - Modellbasierte Arzneimittelentwicklung am Beispiel therapeutischer Proteine.

Systembiologie.de, Ausg. 02, December 2010.

Journal (http://www.systembiologie.de/fileadmin/media/magazine/systembiologie_magazin_ausgabe02.pdf)

A. Y. Weiße, R. Middleton and W. Huisinga.

Quantifying uncertainty, variability and likelihood for ordinary differential equation models.

BMC Systems Biology, 4 (2010).

Journal (<http://dx.doi.org/10.1186/1752-0509-4-144>)(open access)

M. von Kleist, S. Menz and W. Huisinga.

Drug-Class Specific Impact of Antivirals on the Reproductive Capacity of HIV.

PLoS Comput Biol 5 (2010): e1000720.

Journal (<http://dx.doi.org/10.1371/journal.pcbi.1000720>)(open access).

S. Pilari and W. Huisinga.

Lumping of Physiologically Based Pharmacokinetic Models and a Mechanistic Derivation of Classical Compartmental Models.

J. Pharmacokinet. Pharmacodyn. 37 (2010), pp 365-405.

Journal (<http://dx.doi.org/10.1007/s10928-010-9165-1>)

B.-F. Krippendorff, D. Oyarzun and W. Huisinga.

Ligand accumulation counteracts therapeutic inhibition of receptor systems.

Proceedings of Foundations of Systems Biology in Engineering, FOSBE (2009), pp. 173-176.

PDF-Preprint (http://compphysiol.math.uni-potsdam.de/pub/Krippendorff_etal2009_FOSBE-preprint.pdf)

B.-F. Krippendorff, K. Küster, C. Kloft, W. Huisinga.

Nonlinear Pharmacokinetics of Therapeutic Proteins Resulting from Receptor Mediated Endocytosis.

J. Pharmacokinet. Pharmacodyn, 36 (2009), pp 239-260.

Journal (<http://www.springerlink.com/content/c7202j8766080j31/>)(open access), Suppl Material (zip (http://compphysiol.math.uni-potsdam.de/pub/JOPA_2009_RME_SupplementaryMaterial.zip))

B.-F. Krippendorff, R. Neuhaus, P. Lienau, A. Reichel, W. Huisinga.

Mechanism-based Inhibition: Deriving KI and kinact directly from Time-Dependent IC50 Values.

J Biomol Screen. 14 (2009), pp. 913-923.



Journal (<http://dx.doi.org/10.1177/1087057109336751>) PDF-Preprint
(http://compphysiol.math.uni-potsdam.de/pub/Krippendorff_etalPreprint2009_MechanismBasedInhibition.pdf) Suppl
Material (http://compphysiol.math.uni-potsdam.de/pub/Krippendorff_etal2009_MBI-supplement.pdf)

M. von Kleist, and W. Huisinga.

**Pharmacokinetic-Pharmacodynamic relationship of NRTIs and its connection to viral escape:
An example based on Zidovudine.**

Eur J Pharm Sci. 36 (2009), pp. 532-543.

Journal (<http://dx.doi.org/10.1016/j.ejps.2008.12.010>) PDF-Preprint
(http://compphysiol.math.uni-potsdam.de/pub/KleistHuisinga2009_AZT.pdf)

P. Deuflhard, W. Huisinga, T. Jahnke, and M. Wulkow.

Adaptive discrete Galerkin methods applied to the chemical master equation.

SIAM J. Sci. Comput. 30 (2008), pp. 2990-3011.

Journal (<http://dx.doi.org/10.1137/070689759>) PDF-Preprint
(http://compphysiol.math.uni-potsdam.de/pub/Deuflhard_etal2008_CME.pdf)

T. Jahnke, and W. Huisinga.

A dynamical low-rank approach to the chemical master equation.

Bull. Math. Biol. 70 (2008), pp. 2283-2302.

Journal (<http://www.springerlink.com/content/jv816vp348k68u53/>) PDF-Preprint
(http://compphysiol.math.uni-potsdam.de/pub/JahnkeHuisinga2008_DLRA.pdf)

M. von Kleist and W. Huisinga.

**Physiologically based pharmacokinetic modelling: A sub-compartmentalized model of tissue
distribution.**

J. Pharmacokinet. Pharmacodyn. 34 (2007), pp 789-806.

Journal (<http://www.springerlink.com/content/724275515k521675/>) PDF-Preprint
(http://compphysiol.math.uni-potsdam.de/pub/VonKleistHuisinga2007_TissueDistribution.pdf)

S. Rüdiger, J.W. Shuai, W. Huisinga, Ch. Nagaiah, G. Warnecke, I. Parker, M. Falcke.

Hybrid stochastic and deterministic simulations of calcium blips.



Biophys. J. 93 (2007), pp. 1847-1857.

Journal ([http://www.cell.com/biophysj/abstract/S0006-3495\(07\)71442-X](http://www.cell.com/biophysj/abstract/S0006-3495(07)71442-X)) PDF-Preprint
(http://compphysiol.math.uni-potsdam.de/pub/Ruediger_etal_2007_HybridModellingCalciumBlips.pdf)

M. von Kleist, C. Kloft and W. Huisinga.

Combining Systems Biology with physiologically-based pharmacokinetics to support the understanding of drug effects.

Proceedings of Foundations of Systems Biology in Engineering FOSBE (2007), pp. 231-236.

PDF-Preprint (http://compphysiol.math.uni-potsdam.de/pub/VonKleistKloftHuisinga_Fosbe2007.pdf)

T. Jahnke, and W. Huisinga.

Solving the chemical master equation for monomolecular reaction systems analytically.

J. Math. Biol. 54 (2007) pp. 1-26.

Journal (<http://dx.doi.org/10.1007/s00285-006-0034-x>) PDF-Preprint
(<http://compphysiol.mi.fu-berlin.de/pub/JaHu2005MasterEquation.pdf>)

B.-F. Krippendorff, P. Lienau, A. Reichel, W. Huisinga.

Optimizing Classification of Drug-Drug Interaction Potential for CYP450 Isoenzyme Inhibition Assays in Early Drug Discovery.

J Biomol Screen. Vol. 12 (2007), pp. 92-99.

Journal (<http://dx.doi.org/10.1177/1087057106295897>) PDF-Preprint
(<http://compphysiol.math.uni-potsdam.de/pub/TwoPointAssay.pdf>)

R. Telgmann, M. von Kleist, and W. Huisinga.

Software Supported Modelling in Pharmacokinetics.

In 'Computational Life Sciences II', Lecture Notes in Computer Science 4216 (2006), M.R. Berthold, R. Glen, and I. Fischer (Eds.), Springer, pp. 216–225.

Journal (http://dx.doi.org/10.1007/11875741_21) PDF-Preprint
(<http://compphysiol.math.uni-potsdam.de/pub/SoftSuppModell16May06.pdf>)

A. Weiße, I. Horenko, and W. Huisinga.



Adaptive Approach for Modelling Variability in Pharmacokinetics.

In 'Computational Life Sciences II', Lecture Notes in Computer Science 4216 (2006), M.R. Berthold, R. Glen, and I. Fischer (Eds.), Springer, pp. 194-204.

Journal (http://dx.doi.org/10.1007/11875741_19) PDF-Preprint (<http://www.hamilton.ie/compphysiol/pub/ADP16May2006.pdf>)

W. Huisinga, R. Telgmann, and M. Wulkow.

The virtual lab approach to pharmacokinetic: Design principles and concepts.

Drug Discov Today 11(2006) pp. 800-805.

Journal (<http://dx.doi.org/10.1016/j.drudis.2006.07.001>) PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/VirtualLab.pdf>)

A. Alfonsi, E. Cances, G. Turinici, B. Di Ventura and W. Huisinga.

Adaptive simulation of hybrid stochastic and deterministic models for biochemical systems.

ESAIM: Proc. 14 (2005), pp. 1-13.

Journal (<http://www.edpsciences.org/articles/proc/abs/2005/01/alfonsi/alfonsi.html>) PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/AdaptiveHybridSimulation.pdf>)

W. Huisinga and B. Schmidt.

Metastability and Dominant Eigenvalues of Transfer Operators.

In 'Advances in Algorithms for Macromolecular Simulation', Lecture Notes in Computational Science and Engineering 49, C. Chipot, R. Elber, A. Laaksonen, B. Leimkuhler, A. Mark, T. Schlick, C. Schütte, and R. Skeel (Eds.) Springer (2005).

Book (<http://www.springer.com/dal/home/computer/mathematics?SGWID=1-151-22-63370858-0>) PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/MetastabDominantEV.pdf>)

I. Horenko, S. Lorenz, C. Schütte and W. Huisinga.

Adaptive Approach for Non-Linear Sensitivity Analysis of Reaction Kinetics.

J. Comp. Chem. 26 (2005), pp. 941-948.

Journal (<http://www3.interscience.wiley.com/cgi-bin/abstract/110481921/ABSTRACT>) PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/adaptiveSensitivity.pdf>)



K. Abraham, H. Mielke, W. Huisinga and U. Gundert-Remy.

Elevated Internal Exposure of Children in Simulated Acute Inhalation of Volatile Organic Compounds: Dependency on Properties of the Chemical.

Basic & Clinical Pharmacology & Toxicology 96 (2005), pp. 242–243.

Journal (<http://www.blackwell-synergy.com/doi/abs/10.1111/j.1742-7843.2005.pto960315.x>) PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/ChildrenVOCchem.pdf>)

K. Abraham, H. Mielke, W. Huisinga and U. Gundert-Remy.

Elevated Internal Exposure of Children in Simulated Acute Inhalation of Volatile Organic Compounds: Effects of Concentration and Duration.

Arch Toxicol 79 (2005) pp. 63-73.

Journal (<http://www.springerlink.com/index/10.1007/s00204-004-0599-3>) PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/ChildrenVOCtC.pdf>)

Ch. Schütte, J. Walter, C. Hartmann and W. Huisinga.

An Averaging Principle for Fast Degrees of Freedom Exhibiting Long-Term Correlations.

SIAM Multiscale Modeling and Simulation 2 (2004) pp. 501-526.

Journal (<http://epubs.siam.org/sam-bin/dbq/article/60030>) PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/ExtendedAveraging.pdf>)

W. Huisinga, S. Meyn and Ch. Schütte.

Phase Transitions & Metastability in Markovian and Molecular Systems.

Ann. Appl. Probab. 14 (2004), 419-458.

Journal (<http://dx.doi.org/10.1214/aoap/1075828057>) PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/PhaseTransMeta.pdf>)

Ch. Schütte, W. Huisinga and S. Meyn.

Metastability of Diffusion Processes.

Proceeding of the IUTAM Symposium on Nonlinear Stochastic Dynamics (August 26 - August 30, 2002, Illinois/USA), 2003.



Book (<http://www.springeronline.com/sgw/cda/frontpage/0,11855,1-40106-22-33644800-0,00.html>)
PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/IUTAM.pdf>)

W. Huisinga, Ch. Schütte and A. M. Stuart.

Extracting Macroscopic Stochastic Dynamics: Model Problems.

Comm. Pure Appl. Math. 56 (2003),234-269.

Journal (<http://www3.interscience.wiley.com/cgi-bin/abstract/101519806/ABSTRACT>) PDF-Peprint
(<http://compphysiol.math.uni-potsdam.de/pub/ExtractMacroProps.pdf>)

Ch. Schütte and W. Huisinga.

Biomolecular Conformations can be Identified as Metastable Sets of Molecular Dynamics.

in Handbook of Numerical Analysis edited by P. G. Ciarlet, Special Volume: Computational Chemistry (Vol X) ,
guest editor C. Le Bris (2003).

Book (http://www.elsevier.com/wps/find/bookvolume.cws_home/501439/vol10)PDF-Preprint
(<http://compphysiol.math.uni-potsdam.de/pub/BioConfAsMetaSets.pdf>)

Ch. Schütte, W. Huisinga and P. Deuffhard.

Transfer Operator Approach to Conformational Dynamics in Biomolecular Systems.

in "Ergodic Theory, Analysis, and Efficient Simulation of Dynamical Systems" edited by B. Fiedler (2001)
pp.191-223.

Book (<http://www.springeronline.com/sgw/cda/frontpage/0,11855,1-40109-22-2140364-0,00.html>) PDF-Preprint
(<http://compphysiol.math.uni-potsdam.de/pub/danse.pdf>)

Ch. Schütte and W. Huisinga.

Biomolecular Conformations as Metastable Sets of Markov Chains.

Proceedings of the 38th. Annual Allerton Conference on Communication, Control, and Computing, Oct. 4-6,
Allerton House, Monticello, Illinois/USA (2000) pp.1106-1115.

Journal (http://www.elsevier.com/wps/find/bookvolume.cws_home/501439/vol10) PDF-Preprint
(<http://compphysiol.math.uni-potsdam.de/pub/BioConfAsMetaSets.pdf>)

T. Galliat, Wilhelm Huisinga and P. Deuffhard.

Self-Organizing Maps Combined with Eigenmode Analysis for Automated Cluster Identification.



in "Neural Computation" edited by H. Bothe and R. Rojas, ICSC Academic Press (2000) pp.227-232.

PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/SOMs.pdf>)

Ch. Schütte and W. Huisinga.

On Conformational Dynamics induced by Langevin Processes.

in "International Conference on Differential Equations (EquaDiff 99)", edited by B. Fiedler K. Gröger and J. Sprekels, Vol.2 (2000) pp.1247-1262.

Book (<http://www.worldscibooks.com/mathematics/4469.html>)PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/langevin.pdf>)

P. Deuflhard, W. Huisinga, A. Fischer and Ch. Schütte.

Identification of Almost Invariant Aggregates in Reversible Nearly Uncoupled Markov Chains.

Lin. Alg. Appl. 315 (2000) pp. 39-59.

Journal

(http://www.sciencedirect.com/science?_ob=ArticleURL&_udi=B6V0R-40T9J5P-3&_coverDate=08%2F15%2F2000&_ali)

PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/AlmostInvAggregats.pdf>)

W. Huisinga, Ch. Best, R. Roitzsch, Ch. Schütte and F. Cordes.

From Simulation Data to Conformational Ensembles: Structure and Dynamics based Methods.

J. Comp. Chem. , Vol.20 (1999) pp.1760-1774.

Journal (<http://www3.interscience.wiley.com/cgi-bin/abstract/66005872/ABSTRACT>) PDF-Preprint

(<http://compphysiol.math.uni-potsdam.de/pub/SimDataConfEnsemble.pdf>)

Ch. Schütte, A. Fischer, W. Huisinga and P. Deuflhard.

A Direct Approach to Conformational Dynamics based on Hybrid Monte Carlo.

J. Comp. Phys. 151 (1999) pp. 146-168.

Journal

(http://www.sciencedirect.com/science?_ob=ArticleURL&_udi=B6WHY-45N4M0N-7&_coverDate=05%2F01%2F1999&_al)

(<http://compphysiol.math.uni-potsdam.de/pub/ConfDynHMC.pdf>)

W. Huisinga, L. Pesce, R. Kosloff and P. Saalfrank.

Faber and Newton Polynomial Integrators for Open-System Density Matrix Propagation.



J. Chem. Phys., Vol.110 (1999) pp.5538-5547.

Journal (<http://dx.doi.org/10.1063/1.478451>) PDF-Preprint
(<http://compphysiol.math.uni-potsdam.de/pub/Faber.pdf>)

Others:

W. Huisinga.

Using math to optimize medication.

NUI Maynooth Research Magazine, Vol. 1, January 2009.

Research Magazine (<http://communications.nuim.ie/magazine/pdfs/vol01iss01.pdf>)

W. Huisinga.

Computational Physiology.

European Communications in Mathematical and Theoretical Biology, No. 8, January 2006, pp. 12-13.

Journal (<http://www.esmtb.org/communication/ecmtb8.pdf>)

Preprints:

W. Huisinga; 2000.

The Essential Spectral Radius and Asymptotic Properties of Transfer Operators.

PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/EssSpectralRadius.pdf>)

Ch. Schütte, A. Fischer, W. Huisinga and P. Deuflhard

Hybrid Monte Carlo Method for Essential Molecular Dynamics

ZIB Preprint, 1998.

P. Nettesheim, W. Huisinga and Ch. Schütte



Chebyshev Approximation for Wavepacket Dynamics: better than expected

ZIB preprint, 1996

PDF-Preprint (<http://compphysiol.math.uni-potsdam.de/pub/Chebyshev.pdf>)

Theses:

W. Huisinga.

Metastability of Markovian systems: A transfer operator approach in application to molecular dynamics.

PhD thesis in mathematics, Freie Universität Berlin, 2001.

PDF Preprint (<http://compphysiol.math.uni-potsdam.de/pub/HuisingaDiss.pdf>)

W. Huisinga.

Faber-, Newton- und Krylov-Approximation zur Integration grosser Differentialgleichungssysteme aus der Quantenmechanik.

Diploma thesis in mathematics at Free University Berlin, 1997
Awarded by the Deutsche Mathematiker Vereinigung (1998).

PDF-Link (<http://compphysiol.math.uni-potsdam.de/pub/huiDiplom.pdf>)