CURRICULUM VITAE (C3)

Personal/CV VAGU-C3 (25.04.2013)

Name	van Gunsteren, Willem F.
Date of birth	August 7, 1947
Place of birth	Wassenaar, The Netherlands
Nationality	Dutch
Sex	male
Civil Status	married, two children

Address

home	Ratitschweg 13 7212 Seewis Dorf (im Prättigau) Switzerland phone +41-81-325 23 92, +41-79-321 05 40, +31-6-40343276
office	Laboratory of Physical Chemistry ETH Zurich, HCI G237 CH-8093 Zurich Switzerland email: wfvgn@ethz.ch homepage: www.igc.ethz.ch

Education

Institution	*Degree*	*Year*	*Scientific Field*
Free University, Amsterdam	B.Sc.	1968	Physics
Free University, Amsterdam	Meester	1974	Law
Free University, Amsterdam	Ph.D.	1976	Nuclear Physics
University of Groningen	(Postdoc)	1976-1978	Molecular Physics
Harvard University	(Postdoc)	1978-1980	Molecular Physics

Honors

- Doctorate Cum Laude (1976)
- Royal Dutch - Shell Prize for Doctoral Research (1975)
- Royal Dutch Union of Chemists gold medal for research (1987)
- Degussa - Stiftungsgastprofessur für Chemie und Medizin, Johann Wolfgang Goethe - Universität, Frankfurt (1988)
- Visiting Professor, University of Science and Technology of China, Hefei (1993-1997)
- Corresponding member, Royal Dutch Academy of Arts and Sciences (1995)
- 73th Priestly Lecturer Penn State University (1999)
- Visiting Professor, University of Florence (2000)
- 10th Huygens Lecturer Dutch Science Foundation (2001)
- Visiting Professor, University of Leiden (2002)
- Max-Planck Forschungspreis für Chemie und Pharmazie (2002)
- Visiting Professor, École Normale Supérieure, Paris (2007)
- Distinguished Lecturer, CMMS, University of Pittsburgh (2009)
- Golden Tricycle award for most family friendly group leader, ETH Zurich (2009)
- Visiting Professor, University of Natural Resources and Life Sciences, Vienna (2015)

Major research interest

Development of methodology to simulate the behaviour of biomolecular systems

Research and/or Professional Experience

March 1980 - May 1987	Senior Lecturer, Department of Physical Chemistry, University of Groningen, The Netherlands
May 1987 - Sept. 1990	Professor of Physical Chemistry, University of Groningen, The Netherlands
Sept. 1987 - Aug. 1992	Professor of Computational Physics, Free University, Amsterdam, The Netherlands
Nov. 1987 - Sept. 1988	Sabbatical leave, University of California, San Francisco, USA
Sept. 1990 - Jan. 2013	Professor of Computer-Aided Chemistry, ETH Zürich, Zurich, Switzerland
March 1997 - Oct. 1997	Sabbatical leave, University of Oxford, Oxford, U.K.
Jan. 2013 -	Professor Emeritus, ETH Zürich, Zurich, Switzerland
Apr. 2014 - 2018	Ombudsman ETH Zürich, Zurich, Switzerland

Teaching duties

courses on

- Mathematical and Computational Methods in Chemistry
- Statistical Mechanics
- Computational Physics
- Advanced Programming
- Computer Science
- Computer Simulation in Chemistry, Biology and Physics

supervised PhD theses: 48

Organisational experience and duties

- *September 1982*
  one of two organisers of a three-week workshop on nucleotide binding to proteins (15 participants) at CECAM, University of Paris IX, Orsay, France

- *May 1984*
  one of two organisers of a one-week workshop on molecular dynamics and protein structure (140 participants) at the University of North Carolina, Chapel Hill, USA

- *September 1984*

one of two organisers of a three-day CECAM discussion meeting on the design of drugs and vaccines (35 participants) in Amersfoort, The Netherlands

- *August 1985*
  organiser of a three-day CECAM discussion meeting on the calculation of free energy in macromolecular systems (17 participants) in Amersfoort, The Netherlands

- *1986 -*
  Author and organiser of the Groningen Molecular Simulation (GROMOS) software for biomolecular simulation, which is used in hundreds laboratories in more than 60 countries on all continents.

- *1991 -*
  organiser of the yearly international Biomos meeting on biomolecular simulation (30 - 40 participants) at Burg Arras, Germany, as of 2011 in Ausserberg, Switzerland

- *September 1992*
  one of three organisers of a five-day workshop on protein folding and stability (51 participants) in Ascona, Switzerland

- *1993 - 2005*
  Head Competence Centre for Computational Chemistry, Zurich

- *April 1993*
  one of two organisers of a two-day CECAM discussion meeting on the generation of amorphous polymer structures (17 participants) at CECAM, Orsay, France

- *April 1994*
  one of four organisers of a five-day workshop on membranes, theory, simulation and experiment (48 participants) in Ascona, Switzerland

- *1995 - 1997*
  Head Institute of Physical Chemistry, ETH Zurich

- *1997 - 2005*
  President Informatikkommission ETH Zurich

- *November 1997*
  one of nine organisers of a three-day joint workshop of the GDCh and C4 ETHZ on the use of computers in chemistry (93 participants) in Männedorf, Switzerland

- *1997 -*
  Delegate of the President of the ETH for nominations of professors

- *May 1999*
  one of three organisers of a five-day workshop on computational sciences and engineering (80 participants) in Ascona, Switzerland

- *September 1999*
  one of six organisers of a two-day conference on biomolecular structure, dynamics and function (172 participants) in Groningen, The Netherlands

- *2000 - 2002*

Head Department of Chemistry, ETH Zurich (~40M Euro turnover)

- *2001*
  Responsible for festivities regarding the opening of the new chemistry laboratory of the ETH Zurich (~10'000 visitors)

- *2004 – 2014*
  Member of the University Council of the University of Vienna

- *2005*
  Responsible for 150th anniversary festivities of the Department of Chemistry and Applied Biosciences, ETH Zurich (~10'000 visitors)

- *2006-2008*
  Head Department of Chemistry and Applied Biosciences, ETH Zurich (~50M Euro turnover)

- *2006*
  Chair of the Gordon Research Conference on Computational Chemistry (one week with 150 participants) in Les Diablerets, Switzerland

- *2008 - 2013*
  Member Strategiekommission ETH Zurich

- *2009*
  Organiser of a symposium on computational science and engineering (140 participants) in Zurich, Switzerland

- *2014 - 2018*
  Ombudsman of the ETH Zurich

Scientific duties

- Member of the Editorial Board of the European Biophysical Journal
- Founder and Director of a software house for scientific computing software, Biomos b.v., since 1986
- Member of the Editorial Board of the journal Molecular Simulation
- Member of the Editorial Board of the Journal of Biomolecular NMR
- Member of the Editorial Board of the Journal of Computational Chemistry

Invited lectures

1982
- Biophysical Society (Oxford, U.K.)
- Burroughs Wellcome (London, U.K.)
- Rheinisch Westphalische Technische Hochschule (Aachen, Germany)
- University of Alberta (Edmonton, Canada)
- University of California (San Francisco, U.S.A.)
- University of North-Carolina (Chapel Hill, U.S.A.)
- Harvard University (Cambridge, U.S.A.)

1983

- Swedish Agricultural University (Uppsala, Sweden)
- Birkbeck College (London, U.K.)
- Rheinisch Westphalische Technische Hochschule (Aachen, Germany)

1984

- University of Science and Technology of China (Hefei, China)
- Polish Academy of Sciences (Warsaw, Poland)
- University of North Carolina (Chapel Hill, U.S.A.)
- Fysisch Laboratorium, R.U.U. (Utrecht, The Netherlands)

1985

- Institut Laue Langevin (Grenoble, France)
- University of Frankfurt (Frankfurt, Germany)
- Stichting Academisch Rekencentrum Amsterdam (Amsterdam, The Netherlands)
- KNCV (Twente, The Netherlands)
- Royal Swedish Academy of Sciences (Stockholm, Sweden)
- German and Swedish Biophysical Societies (Lübeck, Germany)
- New York Academy of Sciences (New York, U.S.A.)
- Du Pont (Wilmington, U.S.A.)
- KNAW (Amsterdam, The Netherlands)

1986

- Fysisch Laboratorium V.U. (Amsterdam, The Netherlands)
- Molecular Graphics Society (Cap d'Agde, France)
- International Union of Crystallography (Garmisch-Partenkirchen, Germany)

1987

- Molecular Graphics Society (York, U.K.)
- ICI (Macclesfield, U.K.)
- University of Frankfurt (Frankfurt, Germany)
- SON (Lunteren, The Netherlands)
- Material Science Center (Vlieland, The Netherlands)
- Colloquium de Protides (Brussels, Belgium)
- BIOSON (Groningen, The Netherlands)
- Gesellschaft Deutscher Chemiker (Baden-Baden, Germany)
- Unilever (Vlaardingen, The Netherlands)
- Shell (Amsterdam, The Netherlands)
- FEBS (Ljubljana, Yugoslavia)
- Max-Planck Institut für Biochemie (München, Germany)
- Freie Universitat (Berlin, Germany)
- University of Minnesota (Minneapolis, U.S.A.)
- University of Science and Technology of China (Hefei, China)
- University of New South Wales (Sydney, Australia)
- Australian National University (Canberra, Australia)
- Ludwig Institute for Cancer Research (Melbourne, Australia)
- University of Chicago (Chicago, U.S.A.)
- Alliant (Princeton, U.S.A.)

1988

- KNCV (Amsterdam, The Netherlands)
- Bayer (Leverkusen, Germany)
- Florida State University (Tallahassee, U.S.A.)
- UCSD (San Diego, U.S.A.)
- Alliant (Amsterdam, The Netherlands)
- Int. School of Crystallography (Erice, Italy)
- Gordon Research Conf. on Comput. Chemistry (Plymouth, U.S.A.)
- 14th Biochemistry Congress (Prague, Czechoslovakia)
- Molecular Graphics Society (San Francisco, U.S.A.)

- CARB (Rockville, U.S.A.)
- NIH (Bethesda, U.S.A.)
- Du Pont (Wilmington, U.S.A.)
- Wyeth-Ayerst (Princeton, U.S.A.)
- Wesleyan University (Middletown, U.S.A.)
- State University (Utrecht, The Netherlands)
- BASF (Ludwigshafen, Germany)
- Swiss Crystallographic Society (Lausanne, Switzerland)
- Hoffmann-La Roche (Basel, Switzerland)
- Gesellschaft für Biotechnologische Forschung (Braunschweig, Germany)
- J.W. Goethe University (Frankfurt, Germany)
- Hoechst (Frankfurt, Germany)

1989

- University of Oxford (Oxford, U.K.)
- University of Cambridge (Cambridge, U.K.)
- CCP4/CCP5 Meeting, SERC (Daresbury, U.K.)
- Eidg. Technische Hochschule (ETH) (Zurich, Switzerland)
- University of Utrecht (Utrecht, The Netherlands)
- GERM XI (Bordeaux, France)
- Sandoz (Basel, Switzerland)
- ICSN (Gif sur Yvette, France)
- Bio-Expo 89 (Paris, France)
- Int. School of Crystallography (Erice, Italy)
- Alfred Benzon Symposium (Copenhagen, Denmark)
- 32nd IUPAC Congress (Stockholm, Sweden)
- CECAM Meeting (Ermelo, The Netherlands)
- German, Swiss, Austrian and Yugoslavian Biophysical Societies (Todtmoos)
- Alliant (Tokyo, Japan)
- CBI (Tokyo, Japan)
- Philips (Eindhoven, The Netherlands)
- Dutch Biophysical Society (Groningen, The Netherlands)
- Janssen Pharmaceuticals (Tilburg, The Netherlands)
- Technische Universität (München, Germany)
- SON (Lunteren, The Netherlands)

1990

- CECAM Meeting (Orsay, France)
- Rhône-Poulenc (Vitry, France)
- Agricultural University (Wageningen, The Netherlands)
- University of Houston (Houston, U.S.A.)
- Texas A&M University (College Station, U.S.A.)
- Howard Hughes Medical Institute (Dallas, U.S.A.)
- Austrian Chemical Society (Vienna, Austria)
- University of Vienna (Vienna, Austria)
- Biostructure (Strasbourg, France)
- Second Naples Workshop on Bioactive Peptides (Anacapri, Italy)
- DSM (Vaals, The Netherlands)
- C4 Symposium (Zuerich, Switzerland)
- University of Michigan (Ann Arbor, U.S.A.)
- Eli Lilly (Indianapolis, U.S.A.)
- 10th Int. Biophysics Congress (Vancouver, Canada)
- UCSF (San Francisco, U.S.A.)
- 4th Symposium Protein Society (San Diego, U.S.A.)
- IBM Workshop on Polymer Science (Oberlech, Austria)

- European Physical Society (Amsterdam, The Netherlands)
- Czechoslovakian Academy of Sciences (Podebrady, Czechoslovakia)
- Molecular Graphics Society (York, United Kingdom)
- IBM, Intl. Business Machines Corp. (Rüschlikon, Switzerland)
- Eidg. Technische Hochschule (ETH) (Zurich, Switzerland)
- Max-Planck Institut für Biochemie (Martinsried, Germany)
- University of Zurich (Zurich, Switzerland)
- Hoffmann-La Roche (Basel, Switzerland)

1991

- Sandoz (Basel, Switzerland)
- Ciba-Geigy (Basel, Switzerland)
- Ciba Foundation Symposium (London, U.K.)
- Biozentrum University Basel (Basel, Switzerland)
- Dept. Informatik, ETH Zurich (Zurich, Switzerland)
- French Chemical Society (Obernai, France)
- Gesellschaft Deutscher Chemiker (Frankfurt, Germany)
- Swiss Computational Chemists (Bern, Switzerland)
- Dept. Organic Chemistry, University Basel (Basel, Switzerland)
- AKZO (Arnhem, The Netherlands)
- NATO Workshop on Computation in Biotechnology (Sant Feliu, Spain)
- Workshop on Structure and Function of Mutated Proteins (Florence, Italy)
- EMBO Workshop on NMR Structures of Proteins (Kandersteg, Switzerland)
- Workshop on Molecular Simulation (Ovronnaz, Switzerland)
- Gesellschaft für Biologische Chemie (Bayreuth, Germany)
- Ecole Polytechnique (Palaiseau, France)
- CNRS School of Protein Modelling (Toulouse, France)
- Congresso Nazionale die NMR (Milano, Italy)
- 14iemes Journées Scientifiques Rhône-Poulenc (Lyon, France)
- Johannes Gutenberg-Universität Mainz (Mainz, Germany)
- Utrecht Center for Computational Science (Utrecht, The Netherlands)

1992

- Unilever (Vlaardingen, The Netherlands)
- Société Royale de Chimie (Namur, Belgium)
- Rhône-Poulenc Rorer Recherche-Développement (Vitry, France)
- Universität Ulm (Ulm, Germany)
- Workshop on parallel computers (Ascona, Switzerland)
- Cray symposium (Bern, Switzerland)
- Joint Nordic Spring Meeting Physical Societies (Nyborg, Denmark)
- Novo-Nordisk (Bagsvaerd, Denmark)
- Bayer-Pharma (Wuppertal, Germany)
- Dept. Pharmacy ETH Zurich (Zurich, Switzerland)
- Workshop on supercomputing in science and industry (Ascona, Switzerland)
- Gesellschaft Österreichischer Chemiker (Graz, Austria)
- Siemens Nixdorf (München, Germany)
- Colorado State University (Fort Collins, USA)
- 3rd Keck Symposium (Houston, USA)
- Indian Institute of Science (Bangalore, India)
- Dept. Physics, University of Lausanne (Lausanne, Switzerland)
- Unilever (Vlaardingen, The Netherlands)
- Schering (Berlin, Germany)
- Technische Universität (Berlin, Germany)

1993

- Dept. Biochemistry, University of Zurich (Zurich, Switzerland)

- Keystone Symposium 1993 (Taos, USA)
- Workshop on Protein Dynamics & Thermodynamics (Jerusalem, Israel)
- CECAM Workshop on Starting Structures for Polymer Simulation (Paris, France)
- Max-Planck-Institut für Biochemie (Martinsried, Germany)
- Schwerpunktprogramm Informatik Workshop (Bern, Switzerland)
- Agouron Institute (San Diego, USA)
- Nalbandov-Beckman Institute Symposium (Urbana-Champaign, USA)
- Parallel Computational Biology Workshop (Urbana-Champaign, USA)
- Symposium on Macromolecular Structure & Function (Toronto, Canada)
- 12th Annual Conference of the Molecular Graphics Society (Interlaken, Switzerland)
- Société Vaudoise des Sciences Naturelles (Lausanne, Switzerland)
- Zeneca Pharmaceuticals (Macclesfield, United Kingdom)
- 22nd FEBS Meeting (Stockholm, Sweden)
- 7th Rhine-Knee Crystallographers Meeting (Délémont, Switzerland)
- Universitat Polytecnica de Catalunya (Barcelona, Spain)
- Leiden University (Leiden, The Netherlands)

1994

- Unilever Ltd (Vlaardingen, The Netherlands)
- EMBL (Heidelberg, Germany)
- Karolinska Institutet (Stockholm, Sweden)
- Int. Young Scientist meeting on Biotechnology (Ascona, Switzerland)
- Asean Molecular Biology Organisation (Osaka, Japan)
- Protein Engineering Research Institute (Osaka, Japan)
- Chemistry, Biology, Informatics Forum (Tokyo, Japan)
- Protein Engineering and Molecular Design Forum (Tokyo, Japan)
- University of Groningen (Groningen, The Netherlands)
- European Workshop COST-Chemistry (Como, Italy)
- Rhone-Poulenc (Vitry, France)
- 1st Eur. Conf. Comput. Chem. (Nancy, France)
- Ciba-Geigy (Basel, Switzerland)
- Thomae (Biberach, Germany)
- Center for Adv. Res. in Biotechnology (Rockville, USA)
- NIH (Bethesda, USA)
- Univ. of North Carolina (Chapel Hill, USA)
- Rhône-Poulenc/Rorer (Collegeville, USA)
- Bristol-Myers-Squibb (Princeton, USA)
- DuPont-Merck (Wilmington, USA)
- Unilever Ltd. (Vlaardingen, The Netherlands)
- XVI-th Int. Conf. Magn. Res. in Biol. Syst. (Eindhoven, The Netherlands)
- NOVUM Conf. Protein Motion (Stockholm, Sweden)
- Groningen Biomolecular Sciences Institute (Groningen, The Netherlands)
- Royal Society Meeting on Protein Folding (London, U.K.)
- Zeneca Pharmaceuticals (Macclesfield, U.K.)
- Conference at the Institute Juan March (Madrid, Spain)
- Conference at Unilever Ltd. (Vlaardingen, The Netherlands)
- University of Amsterdam (Amsterdam, The Netherlands)

1995

- WISOR IV Winterschool (Bressanone, Italy)
- Chemische Gesellschaft (Fribourg, Switzerland)
- VW-Stiftung Symposium (Hünfeld, Germany)
- University of Florence (Florence, Italy)
- Workshop on Protein Structure (Ripa d'Orcia, Italy)
- 1st Eur. Symp. Protein Society (Davos, Switzerland)

- Eur. Research Conf. NMR in Molecular Biology (Wildbad-Kreuth, Germany)
- University of Heidelberg (Heidelberg, Germany)
- Summerschool on MC and MD simulation (Como, Italy)
- University of Science and Technology of China (Hefei, China)
- National Supercomputing Research Centre of Singapore (Singapore)
- Centre for Math. Modelling and Computer Simulation (Bangalore, India)
- Indian Institute of Science (Bangalore, India)
- C4 Workshop on computational chemistry (Zurich, Switzerland)

1996

- Rhône-Poulenc Rorer (Vitry, France)
- Gesellschaft Deutscher Chemiker (Konstanz, Germany)
- University of Georgia (Athens, USA)
- Genentech, Inc. (South San Francisco, USA)
- 37th ENC Conference (Pacific Grove, USA)
- University of California (San Francisco, USA)
- Agouron Pharmaceuticals (San Diego, USA)
- University of California (San Diego, USA)
- Amgen Inc. (Thousand Oaks, USA)
- University of Zurich (Zurich, Switzerland)
- Gesellschaft österreichischer Chemiker (GÖCH) (Vienna, Austria)
- University of Vienna (Vienna, Austria)
- NATO workshop on biomolecular structure and dynamics (Loutraki, Greece)
- Gordon Research Conference on computational chemistry (New Hampton, USA)
- WATOC '96: 4th World Congress (Jerusalem, Israel)
- IUPAB: 12th Int. Biophys. Congress (Amsterdam, The Netherlands)
- Amer. Chem. Society: 212th National Meeting (Orlando, USA)
- Firmenich S.A. (Geneva, Switzerland)

1997

- Rhône-Poulenc Rorer (Vitry, France)
- Universität Tübingen (Tübingen, Germany)
- Oxford Centre Molecular Sciences (Oxford, U.K.)
- Workshop on computation of protein structure (Oxford, U.K.)
- Dept. Physical Chemistry, University of Oxford (Oxford, U.K.)
- Humboldt Universität (Berlin, Germany)
- 2nd Int. Symp. Algorithms for Macrom. Modelling (Berlin, Germany)
- Givaudan-Roure S.A. (Dübendorf, Switzerland)
- Zeneca Pharmaceuticals (Macclesfield, U.K.)
- IUPAC: 36th Int. Congress (Geneva, Switzerland)
- 3rd Eur. Research Conf. NMR in Molecular Biology (Oxford, U.K.)
- MGS and WATOC Conference: Modelling '97 (Erlangen, Germany)
- 2nd Int. Conf. on Molecular Structural Biology (Vienna, Austria)
- Int. Workshop on Polyelectrolytes, MPI Pol. Forschung (Mainz, Germany)
- 12. CIC Workshop der GDCh (Männedorf, Switzerland)
- Workshop on MC approach to Biopolymers and Folding, KFA (Jülich, Germany)
- Rheinisch-Westphälische Technische Hochschule (Aachen, Germany)
- Int. Workshop on Bioinformatics, Biozentrum, Univ. Basel (Basel, Switzerland)

1998

- Technische Universität München (München, Germany)
- IRRMA simulation course, EPFL (Lausanne, Switzerland)
- Bristol-Myers-Squibb (Princeton, USA)
- Merck-DuPont (Wilmington, USA)
- National Institutes of Health (NIH) (Washington D.C., USA)
- 3rd Johns Hopkins Protein Folding Meeting (Berkeley Springs, USA)

- Eur. Conf. on Comput. Chem. (Chambery, France)
- Biomedical Centre, Uppsala University (Uppsala, Sweden)
- Rhône-Poulenc Rorer (Lyon, France)
- Cours 3ème Cycle en Physique, EPFL (Lausanne, Switzerland)
- CECAM Workshop on implicit solvent models (Lyon, France)
- Symp. on large scale computing, Lund University (Lund, Sweden)
- Cours 3ème Cycle en Physique, EPFL (Lausanne, Switzerland)
- CECAM Workshop on hybrid methods (Lyon, France)
- Gordon Research Conference (Kingston, USA)
- University of Florence (Florence, Italy)
- 6th Naples Workshop on Bioactive Peptides (Capri, Italy)
- EMBO Workshop on Proteins (EMBL, Heidelberg, Germany)
- 34th Symposium for Theoretical Chemistry (Gwatt, Switzerland)
- University of Tübingen (Tübingen, Germany)
- Workshop on protein folding (Madrid, Spain)

1999

- IMS Int. Workshop on Protein Stability and Folding (Okazaki, Japan)
- Oxford Centre Molecular Sciences (Oxford, U.K.)
- Int. School of Struct. Biology and Magn. Resonance (Erice, Italy)
- Gordon Conf. on Comput. Aspects of NMR (Il Ciocco, Italy)
- Kansas State University (Manhattan, USA)
- Workshop on Treatment of Electrostatic Interactions (Santa Fe, USA)
- COST Workshop (Geneva, Switzerland)
- Course Advanced Computing in NMR Spectr. (Florence, Italy)
- Conf. on Understanding Biomol. Struct., Funct., Dyn. (Groningen, The Netherlands)
- Penn State University (State College, USA)
- Univ. of the Sciences in Philadelphia (Philadelphia, USA)
- Univ. of Science and Technology of China (Hefei, China)
- Sino-Swiss Workshop on Bioinformatics (Beijing, China)
- University of Utrecht (Utrecht, The Netherlands)

2000

- National Institute for Medical Research (London, U.K.)
- University of Florence (Florence, Italy)
- 18-th Molecular Graphics Society Meeting (York, U.K.)
- IBM Research Laboratory (Rüschlikon, Switzerland)
- Uppsala University (Uppsala, Sweden)
- VW Symposium on Conformational Control (Kloster Banz, Germany)
- Conference Computational Biophysics 2000 (Nice, France)
- Gordon Research Conference on Biopolymers (Newport, USA)
- IBM Tomas Watson Research Laboratory (Yorktown Heights, USA)
- Gordon Research Conference on Computational Chemistry (Oxford, U.K.)
- University of Barcelona (Barcelona, Spain)
- XIX-th Int. Conf. Magn. Res. in Biol. Sci. (Florence, Italy)
- 7-th Biophysics Summerschool (Rovinj, Croatia)

2001

- University of Massachusetts Medical School (Worcester, USA)
- Wesleyan University (Middletown, USA)
- Bristol-Myers-Squibb (Princeton, USA)
- National Institutes of Health (Bethesda, USA)
- University of California (San Francisco, USA)
- IBM Workshop on Protein Folding (San Diego, USA)
- 221-th ACS meeting (San Diego, USA)
- Annual Meeting Swiss Physical Society (Dübendorf, Switzerland)

- Gesellschaft Deutscher Chemiker (Mülheim, Germany)
- Leiden University (Leiden, The Netherlands)
- Gesellschaft Deutscher Chemiker (Göttingen, Germany)
- Boehringer Ingelheim (Biberach, Germany)
- SIMU conference (Konstanz, Germany)
- University of Queensland (Brisbane, Australia)
- ComBio2001 (Canberra, Australia)
- 7-th Australian Molecular Modelling Workshop (Canberra, Australia)
- Sydney Protein Meeting (Sydney, Australia)
- Ludwig Institute for Cancer Research (Melbourne, Australia)
- NWO/Huygens-lezing (Den Haag, The Netherlands)

2002

- University of Konstanz (Konstanz, Germany)
- Wacker GmbH (München, Germany)
- IBM and NeSC Workshop on Protein Science (Edinburgh, Scotland)
- Lund Life Sciences Symposium (Lund, Sweden)
- Symposium New Chemistry ETH Zurich (Zurich, Switzerland)
- University of Pernambuco (Recife, Brazil)
- Workshop on Modeling in Biophysics (Rio de Janeiro, Brazil)
- University of Sao Paulo (Sao Paulo, Brazil)
- University of Sao Paulo (Ribeirao Preto, Brazil)
- University of Leiden (Leiden, The Netherlands)
- COST-D9 Workshop (Smolenice, Slovakia)
- University of Groningen (Groningen, The Netherlands)
- Gordon Research Conf. on Comput. Chemistry (New London, USA)
- SFC Eurochem Conference (Toulouse, France)
- Exploring Modern Comput. Chemistry (Nottingham, UK)
- WATOC'02 (Lugano, Switzerland)
- Bijvoet Seminar, University of Utrecht (Utrecht, The Netherlands)
- Ehrenfest Colloquium, University of Leiden (Leiden, The Netherlands)
- 44th Symp. of Soc. for Histochemistry (Vlissingen, The Netherlands)
- NCCR Symposium Uni Zurich (Zurich, Switzerland)

2003

- Sharif University of Technology (Tehran, Iran)
- University of Tehran (Tehran, Iran)
- Tarbiat Modarres University (Tehran, Iran)
- University of Leiden (Leiden, The Netherlands)
- University of Bordeaux (Bordeaux, France)
- 7th Annual Meeting Swedish Structural Biology (Tallberg, Sweden)
- Summerschool Biomolecular Structure and Dynamics (Otočec, Slovenia)
- Astra Zeneca (Macclesfield, U.K.)
- Oxford University (Oxford, U.K.)
- 11th Intl. Congress of Quantum Chemistry (Bonn, Germany)
- Technical University Delft (Delft, The Netherlands)
- 8th Biophysics Summerschool (Rovinj, Croatia)
- National Institutes of Health (Bethesda, USA)

2004

- Conf. on Theory and Applic. of Comput. Chemistry (Gyeongju, S.Korea)
- ETH-Kolloquium Naturwiss. und Unterricht (Zurich, Switzerland)
- Free University (Amsterdam, The Netherlands)
- Workshop Intrinsic Reactivity of New Molec. Materials (Nice, France)
- Intl. Meeting Molec. Graphics and Modelling Society (Manchester, U.K.)
- EMBO Course Methods for Protein Simulation and Drug Design (Shanghai, China)

- University of Science and Technology of China (Hefei, China)
- University of Beijing (Beijing, China)
- 2nd Eur. Conf. on Chemistry towards Biology (Seggau/Graz, Austria)
- Pantok Dialogos (Zurich, Switzerland)

2005

- WATOC Congress (Capetown, South Africa)
- Kolloquium Naturwiss. at University Basel (Basel, Switzerland)
- Glaxo-Smith-Kline (Stevenage, UK)
- Pfizer (Sandwich, UK)
- Royal Dutch Acad. Sciences (Amsterdam, The Netherlands)
- Symposium Frontiers in Comput. Biology, NIH (Washington, USA)
- Kolloquium Phys. Chemie ETH (Zurich, Switzerland)
- Dutch Polymer Institute, Tech. Univ. Eindhoven (Eindhoven, The Netherlands)
- Sika Technologies AG, (Zurich, Switzerland)
- Boehringer (Wien, Austria)
- Symposium Theoretical Chemistry (Innsbruck, Austria)
- Parrinello Symposium (Monte Verita, Ascona, Switzerland)
- FEBS Course Theo. Mod. of ligand binding and enzymatic catalysis (Tromsö, Norwegen)
- Intl. Conf. on Diff. Eq. from Theory to Comput. Sci. and Eng. (Zurich, Switzerland)
- Rotary Club (Zug, Switzerland)
- Conf. Biol. Dynamics: from molecules to cells (Amsterdam, The Netherlands)

2006

- Chemische Gesellschaft Darmstadt (Darmstadt, Germany)
- Univ. Heidelberg (Heidelberg, Germany)
- Organon N.V. (Oss, The Netherlands)
- University of Vienna (Vienna, Austria)
- Technical University of Munich (Munich, Germany)
- Kolloquium Rechnergestützte Wissenschaften, ETH Zurich (Zurich, Switzerland)
- University of Basel (Basel, Switzerland)
- Max Gruber Lecture, University of Groningen (Groningen, The Netherlands)
- University of Ljubljana (Ljubljana, Slovenia)
- Summer school Varenna (Varenna, Italy)
- 1st European Chemistry Congress (Budapest, Hungary)
- IFPSC Workshop, 3M Headquarters (St Paul, USA)

2007

- J. W. Goethe University (Frankfurt, Germany)
- University of Leiden (Leiden, The Netherlands)
- University of Heidelberg (Heidelberg, Germany)
- Ecole Normale Superieure (Paris, France)
- Institut de Biologie Physico-Chimique (Paris, France)
- Darmstädter Molecular Modelling Workshop (Erlangen, Germany)
- BIG seminar series, University Lausanne (Lausanne, Switzerland)
- Bioinformatics Institute, Biomed. Res. Council (Singapore)
- Nanyang Technical University (Singapore)
- National Institute of Chemistry (Ljubljana, Slovenia)
- Rudjer Boskovic Institute (Zagreb, Slovenia)
- Course on free energy calculation (Zurich, Switzerland)
- 12th European Conf. on the spectroscopy of biological molecules (Bobigny, France)
- Conference on biomolecular simulation and experiment (Manchester, UK)
- University of Leeds (Leeds, UK)
- University of Oxford (Oxford, UK)
- Birkbeck College, University of London (London, UK)
- Symposium on light-induced dynamics of biopolymers (Munich, Germany)

2008

- 6th NCCR course on biomolecular modelling (Kandersteg, Switzerland)
- Zing conference on computational biophysics (Antigua and Barbuda)
- Kolloquium Rechnergestützte Wissenschaften, ETH (Zurich, Switzerland)
- CASP 7.5 conference (Madrid, Spain)
- Ludwig-Maximilians University (Munich, Germany)
- Theoretical Biochemistry Conference (Stockholm, Sweden)
- Workshop Computational Biology and System Biology (Jülich, Germany)
- Pfizer Ltd. (Sandwich, UK)
- NCCR structural biology seminar (Zurich, Switzerland)
- National Yang-Ming University (Taipei, Taiwan)
- Academica Sinica (Taipei, Taiwan)
- Biomolecular Modelling Retreat (Stradbroke Island, Australia)
- WATOC conference (Sydney, Australia)
- TACC conference (Shanghai, China)
- University of Science and Technology of China (Hefei, China)
- CAS-SSSTC workshop (Zurich, Switzerland)

2009

- Deutsche Chemische Gesellschaft (Berlin, Germany)
- University of Chicago (Chicago, USA)
- Cornell Medical College (New York, USA)
- University of Pittsburgh (Pittsburgh, USA)
- Department of Chemistry, University of Vienna (Vienna, Austria)
- Academy of Science (Linz, Austria)
- Department of Physics, University of Vienna (Vienna, Austria)
- Boehringer GmbH (Vienna, Austria)
- Theoretical and Computational chemistry, University of Vienna (Vienna, Austria)
- Department of Physics, University of Rome La Sapienza (Rome, Italy)
- Biomolecular Simulation Workshop (Stockholm, Sweden)
- 23rd Symposium of the Protein Society (Boston, USA)
- Mediterranean Institute for Life Sciences (Split, Croatia)
- 3rd Adriatic Meeting on Computational Solutions in the Life Sciences (Primosten, Croatia)
- Symp. Frontiers in Macromol. Simulation (Atlanta, USA)

2010

- 8th NCCR course on biomolecular modelling (Kandersteg, Switzerland)
- King's College, University London (London, UK)
- Int. Symp. Theoretical and Comput. Chemistry (Muelheim, Germany)
- Workshop Frontiers in the Life Sciences (Strasbourg, France)
- University of Calgary (Calgary, Canada)
- University of Alberta (Edmonton, Canada)
- ACS - meeting (San Francisco, USA)
- Sino Swiss courses on biomolecular modelling (Hefei, China)
- Chinese Academy of Sciences (Beijing, China)
- Tsinghua University (Beijing, China)
- Int. Soc. Quant. Biology & Pharmacy (Cetraro, Italy)
- Gordon Conf. Comput. Chemistry (Les Diablerets, Switzerland)
- 8-th NCCR Symposium on Structural Biology (Zurich, Switzerland)
- Inst. St. Raffaele (Milano, Italy)
- CECAM workshop on Protein Folding (Lausanne, Switzerland)
- Symp. Frontiers in Simulation (Los Angeles, USA)

2011

- University Göttingen (Göttingen, Germany)
- MPI for Biophysical Chemistry (Goettingen, Germany)

- Univ. Nat. Sci. Vienna (Vienna, Austria)
- Uppsala University (Uppsala, Sweden)
- PSI (Villigen, Switzerland)
- IIQB (Oeiras, Portugal)
- CECAM workshop on thermodynamics (Palaiseau, France)
- LPC colloquium ETH (Zurich, Switzerland)
- GDCh colloquium (Karlsruhe, Germany)
- Biochemical Summerschool (Spetses, Greece)
- University of Cape Town (Cape Town, South Africa)
- WATOC 2011 (Santiago de Compostela, Spain)
- 47-th Symp. Theor. Chemistry (Sursee, Switzerland)
- 2nd Workshop on Molecular Kinetics (Berlin, Germany)

2012

- 10th NCCR course on biomolecular modelling (Kandersteg, Switzerland)
- Karolinska Institut (Stockholm, Sweden)
- Biotop seminar, Universität für Bodenkultur (Vienna, Austria)
- 10th NCCR Symposium on Structural Biology (Zurich, Switzerland)
- Danube Center for Atomistic Modeling (Vienna, Austria)
- Promotionsfeier ETH Zürich (Zurich, Switzerland)

2013

- 57th General meeting Biophysical Society (Philadelphia, USA)
- DECHEMA workshop on modelling and simulation (Frankfurt, Germany)
- ACS meeting (New Orleans, USA)
- University of Salerno (Salerno, Italy)
- Farewell lecture ETH Zürich (Zurich, Switzerland)
- University of Leipzig (Leipzig, Germany)
- Symposium Computers in Chemistry (Amsterdam, The Netherlands)
- Workshop on free energy calculations (Snowmass, USA)
- Conference Particles 2013 (Stuttgart, Germany)
- Workshop on protein dynamics (Saig, Germany)
- University of Cape Town (Cape Town, South Africa)
- HITS Heidelberg (Heidelberg, Germany)
- Federal University of Pernambuco (Recife, Brazil)
- University of Sao Paulo (Sao Paulo, Brazil)
- 17th Braz. Symp. Theor. Chem. (Angra dos Reis, Brazil)
- Pontifical Catholic University (Rio de Janeiro, Brazil)

2014

- CECAM Workshop on Proteins (Stuttgart, Germany)
- CECAM Workshop on Entropy (Vienna, Austria)
- FEBS Course on Ligand-Protein Binding (Nové Hrady, Czechia)
- Gesellschaft Deutscher Chemiker, University of Konstanz (Konstanz, Germany)
- Bioinformatics Institute A-star (Singapore)
- Students and Early-Career Research Forum, Lamington Natl. Park (Queensland, Australia)
- Molecular Modelling Conf. AMMA2014, Lamington Natl. Park (Queensland, Australia)
- IUPAB Conference 2014 (Brisbane, Australia)
- University of Hong Kong (Hong Kong, China)
- Diskussions Forum Sternwarte ETH (Zurich, Switzerland)

2015

- ACS meeting (Denver, USA)
- Course on Molecular Modelling at the Bodenkulturuniversität Wien (Vienna, Austria)
- Advanced School Biomolecular Simulation (Recife, Brazil)
- Biophysical Society of Brazil (Natal, Brazil)
- Gordon Research Seminar (Il Ciocco, Italy)

- CANES Annual Retreat (Windsor, U.K.)
- Conference on Validation of Simulation (Hannover, Germany)
- Dept. Chemistry and Pharmacy, Free University (Amsterdam, The Netherlands)
- SMASH 2015 NMR conference (Baveno, Italy)
- Paul Scherrer Institute (Villigen, Switzerland)
- Workshop Proteins and Beyond, Leiden University (Leiden, The Netherlands)
- Amsterdam Institute for Molecules, Medicines and Systems (Amsterdam, The Netherlands)
- Practical Course in Biomolecular Modelling, AIMMS (Amsterdam, The Netherlands)
- Centro Interdisciplinario de Neurocienca de Valparaiso (Valparaiso, Chile)
- Int. Spring School Thermodynamics, Fondación Cienca & Vida (Santiago de Chile, Chile)

2016

- Workshop on Polarisation, University of British Columbia (Vancouver, Canada)
- University of Vienna (Vienna, Austria)
- Intl. Conf. on Molecular Simulation, ICMS2016 (Shanghai, China)
- ChemPartner CRO (Shanghai, China)

2017

- University of Alberta (Edmonton, Canada)
- CECAM Workshop on Comput. Challenges in Drug Discovery (Lausanne, Switzerland)
- MIM Workshop on Laboratory Management (Zürich, Switzerland)
- Rechtswissenschaftliches Institut Universität Zürich (Zürich, Switzerland)
- Int. Spring School Thermodynamics, Fondación Cienca & Vida (Santiago de Chile, Chile)

2018

- CECAM Workshop on Analysis and Design of Allostery (Lausanne, Switzerland)
- Swiss Academy of Sciences (SCNAT): “Young Faculty Meeting” (Bern, Switzerland)
- Swiss Academy of Sciences (SCNAT): “Ethics in Chemistry” (Fribourg, Switzerland)

2019

- Lorentz-CECAM Summerschool on Multi-Scale Modelling (Leiden, The Netherlands)
- CECAM Summerschool “Introduction to Biomolecular Simulation” (Vienna, Austria)
- Leopoldina Jahresversammlung: “Zeit in Natur und Kultur” (Halle, Germany)

2020

- None, due to the corona pandemic

2021

- None, due to the corona pandemic

2022

- None, due to the corona pandemic

Scientific publications, books

Date: 02-10-2022

Edited:

- W.F. van Gunsteren, P.K. Weiner, eds.
  Computer Simulation of Biomolecular Systems,
  Theoretical and Experimental Applications,
  Escom Science Publishers, Leiden, The Netherlands, 1989, 224 pages
  ISBN 90-72199-03-0

- W.F. van Gunsteren, P.K. Weiner, A.J. Wilkinson, eds.
  Computer Simulation of Biomolecular Systems,
  Theoretical and Experimental Applications, Vol. 2,
  Escom Science Publishers, Leiden, The Netherlands, 1993, 589 pages
  ISBN 90-72199-15-4

- W.F. van Gunsteren, P.K. Weiner, A.J. Wilkinson, eds.
  Computer Simulation of Biomolecular Systems,
  Theoretical and Experimental Applications, Vol. 3,
  Kluwer Academic Publishers, Dordrecht, The Netherlands, 1997, 618 pages
  ISBN 90-72199-25-1

Authored:

- W.F. van Gunsteren, S.R. Billeter, A.A. Eising, P.H. Hünenberger, P. Krüger, A.E. Mark, W.R.P. Scott, I.G. Tironi
  Biomolecular Simulation: The GROMOS96 Manual and User Guide
  Vdf Hochschulverlag AG an der ETH Zürich, Zürich, Switzerland, 1996, 1042 pages
  ISBN 3 7281 2422 2

Scientific publications, articles

1. W.F. van Gunsteren, E. Boeker, K. Allaart
The FBCS model and the inverse gap equations applied to the tin isotopes
Z. Phys. **267** (1974) 87-96

2. K. Allaart, W.F. van Gunsteren
Projected quasiparticle calculations in large model spaces
Nucl. Phys. **A234** (1974) 53-60

3. W.F. van Gunsteren, K. Allaart
Can the o^+ states of even superfluid nuclei be described by anharmonic pairing vibrations ?
Nucl. Phys. **A236** (1974) 317-326

4. W.F. van Gunsteren, K. Allaart
Influence of an enlargement of the model space on number projected quasiparticle calculations
Z. Phys. **A276** (1976) 1-8

5. W.F. van Gunsteren, K. Allaart, E. Boeker
A particle-quasiparticle description of ^{112,114,116}Sb
Nucl. Phys. **A266** (1976) 365-378

6. W.F. van Gunsteren
A hole-quasiparticle description of ^{114,116}In
Nucl. Phys. **A265** (1976) 263-279

7. W.F. van Gunsteren, P. Hofstra, H. Muether
Influence of the effective interaction on spectra of superfluid nuclei
Z. Phys. **A278** (1976) 251-255

8. W.F. van Gunsteren
The nuclear quasiparticle model
Thesis, Vrije Universiteit Amsterdam, 1976, 253 pag.

9. W.F. van Gunsteren, D. Rabenstein
Properties of the low-lying levels of ^{122}Sb
Z. Phys. **A282** (1977) 55-64

10. W.F. van Gunsteren, H.J.C. Berendsen
Algorithms for macromolecular dynamics and constraint dynamics
Mol. Phys. 34 (1977) 1311-1327

11. W.F. van Gunsteren, K. Allaart, P. Hofstra
Number-projected three-quasiparticle description of the odd Sn isotopes
Z. Phys. **A288** (1978) 49-57

12. W.F. van Gunsteren, H.J.C. Berendsen, J.A.C. Rullmann
Inclusion of Reaction Fields in Molecular Dynamics: Application to Liquid Water
Faraday Disc. Chem. Soc. **66** (1978) 58-70

13. T. Lee, J. Bisschop, W. van der Lugt, W.F. van Gunsteren
Radial distribution functions of liquid Na and Cs
Physica **93B** (1978) 59-62

14. W.F. van Gunsteren
Constrained dynamics of flexible molecules
Mol. Phys. **40** (1980) 1015-1019

15. W.F. van Gunsteren, M. Karplus
A Method for Constrained Energy Minimization of Macromolecules
J. Comput. Chem. **1** (1980) 266-274

16. W.F. van Gunsteren, H.J.C. Berendsen, J.A.C. Rullmann
Stochastic dynamics for molecules with constraints Brownian dynamics of n-alkanes
Mol. Phys. **44** (1981) 69-95

17. W.F. van Gunsteren, M. Karplus
Effect of constraints, solvent and crystal environment on protein dynamics
Nature **293** (1981) 677-678

18. H.J.C. Berendsen, J.P.M. Postma, W.F. van Gunsteren, J. Hermans
Interaction models for water in relation to protein hydration
In: "Intermolecular Forces", B. Pullman ed., Reidel, Dordrecht, 1981, p. 331-342

19. W.F. van Gunsteren, M. Karplus
Effect of Constraints on the Dynamics of Macromolecules
Macromolecules **15** (1982) 1528-1544

20. W.F. van Gunsteren, M. Karplus
Protein Dynamics in Solution and in a Crystalline Environment: A Molecular Dynamics Study
Biochemistry **21** (1982) 2259-2274

21. W.F. van Gunsteren, H.J.C. Berendsen
Algorithms for brownian dynamics
Mol. Phys. **45** (1982) 637-647

22. W.F. van Gunsteren, H.J.C. Berendsen
On the fluctuation-dissipation theorem for interacting brownian particles
Mol. Phys. **47** (1982) 721-723

23. W.F. van Gunsteren, H.J.C. Berendsen
Molecular dynamics: perspective for complex systems
Biochem. Soc. Trans. **10** (1982) 301-305

24. S. Swaminathan, T. Ichiye, W.F. van Gunsteren, M. Karplus
Time Dependence of Atomic Fluctuations in Proteins: Analysis of Local and Collective Motions in Bovine Pancreatic Trypsin Inhibitor
Biochemistry **21** (1982) 5230-5241

25. W.F. van Gunsteren, H.J.C. Berendsen, J. Hermans, W.G.J. Hol, J.P.M. Postma
Computer simulation of the dynamics of hydrated protein crystals and its comparison with X-ray data
Proc. Natl. Acad. Sci USA **80** (1983) 4315-4319

26. M. Karplus, S. Swaminathan, T. Ichiye, W.F. van Gunsteren
Local and collective motions in protein dynamics
In: "Mobility and function in proteins and nucleic acids",
Ciba Symp. **93**, Pitman, London, (1983), pp. 271-290

27. W.F. van Gunsteren, H.J.C. Berendsen
Stochastic dynamics of polymers
In: "The Physics of Superionic Conductors and Electrode Materials", J.W. Perram, ed.,
NATO ASI Series **B92** (1983) 241-256 (Plenum Press)

28. H.J.C. Berendsen, W.F. van Gunsteren
Molecular dynamics with constraints
In: "The Physics of Superionic Conductors and Electrode Materials", J.W. Perram, ed.,
NATO ASI Series **B92** (1983) 221-240 (Plenum Press)

29. J. Hermans, H.J.C. Berendsen, W.F. van Gunsteren, J.P.M. Postma
A Consistent Empirical Potential for Water-Protein Interactions
Biopolymers **23** (1984) 1513-1518

30. H.J.C. Berendsen, W.F. van Gunsteren
Molecular Dynamics Simulations: Techniques and Approaches
In: "Molecular Liquids – Dynamics and Interactions", A.J. Barnes et al. eds.,
NATO ASI Series **C135** (1984) 475-500 (Reidel, Dordrecht)

31. W.F. van Gunsteren, H.J.C. Berendsen
Computer Simulation as a Tool for Tracing the Conformational Differences between Proteins in Solution and in the Crystalline State
J. Mol. Biol. **176** (1984) 559-564

32. W.F. van Gunsteren, H.J.C. Berendsen, F. Colonna, D. Perahia, J.P. Hollenberg, D. Lellouch
On Searching Neighbours in Computer Simulations of Macromolecular Systems
J. Comput. Chem. **5** (1984) 272-279

33. H.J.C. Berendsen, W.F. van Gunsteren, J.P.M. Postma
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In: "High-Speed Computation", J.S. Kowalik, ed.,
NATO ASI Series **F7** (1984) 425-438 (Springer, Berlin)

34. H.J.C. Berendsen, J.P.M. Postma, W.F. van Gunsteren, A. DiNola, J.R. Haak
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35. W.F. van Gunsteren, R. Kaptein, E.R.P. Zuiderweg
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36. K. Remerie, W.F. van Gunsteren, J.P.M. Postma, H.J.C. Berendsen, J.B.F.N. Engberts
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Mol. Phys. **53** (1984) 1517-1526

37. R. Kaptein, E.R.P. Zuiderweg, R.M. Scheek, R. Boelens, W.F. van Gunsteren
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J. Mol. Biol. **182** (1985) 179-182

38. K. Remerie, W.F. van Gunsteren, J.B.F.N. Engberts
Molecular dynamics computer simulation as a tool for the analysis of solvation. A study of dilute aqueous solutions of 1,4-dioxane and 1,3-dioxane
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39. J. Åqvist, W.F. van Gunsteren, M. Leijonmarck, O. Tapia
A Molecular Dynamics Study of the C-terminal Fragment of the L7/12 Ribosomal Protein. Secondary Structure Motion in a 150 Picosecond Trajectory
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40. E.R.P. Zuiderweg, R.M. Scheek, R. Boelens, W.F. van Gunsteren, R. Kaptein
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41. B. Witholt, W.F. van Gunsteren, W.G.J. Hol
Protein Engineering
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42. W.F. van Gunsteren, H.J.C. Berendsen
Molecular Dynamics Simulations: Techniques and Applications to Proteins
In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558,USA, (1985), pp. 5-14

43. H.J.C. Berendsen, J.P.M. Postma and W.F. van Gunsteren
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In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 43-46

44. W.F. van Gunsteren, R. Boelens, R. Kaptein, R.M. Scheek, E.R.P. Zuiderweg
An Improved Restrained Molecular Dynamics Technique to Obtain Protein Tertiary Structure from Nuclear Magnetic Resonance Data
In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 92-99

45. I. Haneef, I.D. Glover, I.J. Tickle, D.S. Moss, S.P. Wood, T.L. Blundell, W.F. van Gunsteren
The Dynamics of Pancreatic Polypeptide: A Comparison of X-ray Anisotropic Refinement at 0.98 K Resolution, Molecular Dynamics and Normal Mode Analysis
In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 85-91

46. J. Äqvist, W.F. van Gunsteren, M. Leijonmarck, O. Tapia
A Molecular Dynamics Study of the C-terminal Fragment of the L7/L12 Ribosomal Protein
In: "Molecular Dynamics and Protein Structure", J. Hermans ed., Polycrystal Book Service, P.O. Box 27, Western Springs, Ill. 60558, USA, (1985), pp. 145-147

47. H. Kessler, B. Kutscher, R. Kerssebaum, A. Klein, J. Lautz, R. Obermeier, H. Muellner, W.F. van Gunsteren, R. Boelens, R. Kaptein
Design, synthesis and conformation of superactive thymopoietin-analogues
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48. W.F. van Gunsteren, H.J.C. Berendsen, J.P. Hollenberg
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49. P. Kruger, W. Strassburger, A. Wollmer, W.F. van Gunsteren
A comparison of the structure and dynamics of avian pancreatic polypeptide hormone in solution and in the crystal
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50. K. Remerie, W.F. van Gunsteren, J.B.F.N. Engberts
A molecular dynamics computer simulation study of the hydration of bis(methylsulfonyl)methane in water
Mol. Phys. **56** (1985) 1393-1409

51. R.M. Scheek, E.R.P. Zuiderweg, R. Boelens, W.F. van Gunsteren, R. Kaptein
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52. H.J.C. Berendsen, W.F. van Gunsteren
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53. K. Remerie, J.B.F.N. Engberts, W.F. van Gunsteren
A molecular dynamics computer simulation study of the temperature dependence of hydration of 1,4-dioxane and 1,3-dioxane
Chemical Physics **101** (1986) 27-44

54. W.F. van Gunsteren, H.J.C. Berendsen, R.G. Geurtsen, H.R.J. Zwinderman
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55. H.J.C. Berendsen, W.F. van Gunsteren, H.R.J. Zwinderman, R.G. Geurtsen
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56. W.F. van Gunsteren
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57. P. Sandblom, J. Äqvist, T.A. Jones, M.E. Newcomer, W.F. van Gunsteren, O. Tapia
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58. J. de Vlieg, R. Boelens, R.M. Scheek, R. Kaptein, W.F. van Gunsteren
Restrained Molecular Dynamics Procedure for Protein Tertiary Structure Determination from NMR Data: A *Lac* Repressor Headpiece Structure Based on Information on J-coupling and from Presence and Absence of NOE's
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59. J. Äqvist, P. Sandblom, T.A. Jones, M.E. Newcomer, W.F. van Gunsteren, O. Tapia
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Eur. Biophys. J. **16** (1988) 153-168

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Research by Wilfred F. van Gunsteren since 1972

(02/10/2022)

Since 1972 Wilfred van Gunsteren (WFvG) has been active in research, till 1976 in computational nuclear physics at the Free University of Amsterdam, after that year in computer simulation of bio-molecular systems at the University of Groningen (1976-1978, 1980-1990), at Harvard University (1978-1980), and at the ETH in Zürich (Swiss Federal Institute of Technology) since 1990. His major research interest is the development of methodology to simulate the behaviour of bio-molecular systems, in particular proteins [e.g. paper 402]. By applying the developed methodology to bio-molecular systems of practical interest, for which ample experimental data are available, deficiencies of current methodology can be identified and new ideas may emerge. Simulation of bio-molecular systems per se leads to enhanced insight into bio-molecular processes at the atomic level, which are often inaccessible to experimental probes. Below the major research activities are briefly sketched. The references to publications are coded according to the publication list of WFvG.

1. Molecular dynamics simulation: general algorithmic developments

- Molecular dynamics (MD) time integration algorithms for harmonic versus non-harmonic forces [10].
- MD simulation at constant temperature and pressure [34].
- A method to simulate molecular systems at constant chemical potential [176].
- A method to simulate molecular systems at constant pH [326].
- Use of bond, bond-angle or dihedral-angle constraints in large molecules [10,14,15,16,19,28,294,407,609,611,616].
- A method to impose flexible (adiabatic) constraints in MD simulation [388,427].
- Searching neighbour particles in simulations of macromolecular systems [32].
- Multiple-time-step algorithms for MD simulation [54,99,337,612,615].
- Time integration algorithms for stochastic dynamics (SD) simulation [21,22,27,71].
- An improved leap-frog kinetic energy expression [437].
- MD simulation in four dimensions [147,165].
- Methods to calculate the dielectric permittivity of liquids [306,504].
- Multi-graining: an algorithm for simultaneous fine-grained and coarse-grained simulation [409].
- Use of weak-coupling in replica-exchange simulation [590].
- An algorithm for flexible boundaries in multi-resolution simulation [594].

2. Atomic-level (GROMOS) force-field development for bio-molecular systems

- Force-field parametrisation using the weak-coupling method [181,191].
- Force-field parametrisation using quasi-Newtonian dynamics for the parameters [227].
- Force-field parameters for protein-water interactions [29].
- GROMOS force field 43A1 for bio-molecular simulation [243,254].
- GROMOS force field 43A2 for bio-molecular simulation [284].
- GROMOS force field 45A3 for bio-molecular simulation [304,339].
- GROMOS force field 45A4 for bio-molecular simulation [371].
- GROMOS force field 53A5 and 53A6 for bio-molecular simulation [358].
- GROMOS force field 54A7 and 54B7 for bio-molecular simulation [470,507].

- GROMOS force field 54A7_ß and 54B7_ß for beta-peptides [505,570].
- Flexible versus rigid models of liquids [213].
- A simple point-charge model (SPC) for liquid water [18,324,340,497,581].
- Model for chloroform [173,487,527].
- Model for dimethyl sulfoxide [189,349,527,577].
- Model for carbon tetrachloride [223,496].
- Model for methanol [276,406,527].
- Model for urea [348,586].
- Model for acetonitrile [393].
- Model for ethylene glycol [432].
- Model for dimethyl sulfone [516].

3. Treatment of (long-range) electrostatic interactions in molecular simulation

- Inclusion of the (stochastic and delayed) electrostatic reaction-field in simulations [12,192,230].
- Analysis of the P3M method to calculate long-range electrostatic interactions [177,196].
- Method to calculate non-periodic long-range electrostatic interactions using P3M [211].
- Different schemes to incorporate long-range forces in MD simulation [245,300,342].
- Method to calculate dielectric permittivity and relaxation [504].

4. Mean-solvation force-field terms

- Stochastic and frictional forces representing the omitted solvent degrees of freedom [78].
- Mean-solvation models for simulation of proteins in water [214,500,545,617].

5. Introduction of polarisability into molecular force fields

- Development of a charge-on-spring (COS) model for polarisability in MD simulation [436,465,579].
- A polarisable model for liquid water [338,365,465,579,581].
- A polarisable model for liquid methanol and methanol-water mixtures [406].
- A polarisable model for liquid ethylene glycol and ethylene glycol-water mixtures [432].
- A polarisable model for chloroform [487].
- A polarisable model for carbon tetrachloride [496].
- A polarisable model for liquid hydrocarbons [574].
- A polarisable model for dimethyl sulfoxide and dimethyl sulfoxide-water mixtures [577].
- A polarisable model for urea-water mixtures [586].
- A polarisable model for acetone [597].

6. Supra-atomic/molecular-level (GROMOS) force-field development for bio-molecular systems

- Using a too large time step in MD simulation of supra-atomic coarse-grained models [457,473].
- A supra-molecular polarisable model for liquid water [497,533].
- Supra-molecular polarisable models for dimethyl sulfoxide, chloroform and methanol [527].
- Mixed fine-grained (atomic) and coarse-grained (supra-molecular) systems [533,534,536,555,575,583].

- A supra-atomic polarisable model for alkanes [588,591].

7. Searching and sampling the (vast) configuration space of large bio-molecules

- Conformational search by potential energy annealing [112].
- Local-elevation: a method to improve the searching of conformational space [174].
- Conformational search using a Boltzmann-weighted mean-field approach [219].
- Conformational search by cooperative MD simulation [249].
- Sampling rare events using hidden restraints [407].
- Adiabatic decoupling of degrees of freedom to enhance configurational sampling [502,510,513,529].
- Enhanced conformational sampling using EDS [569].

8. Structure determination or refinement of proteins based on experimentally derived data

- Determination of protein structure from NMR data using restraining MD simulation [35,37,40,44].
- Time-dependent NOE distance restraints in protein structure determination by NMR [89,96].
- Time-dependent restraints in protein structure determination by X-ray diffraction [98,140,180,265].
- Time-dependent ^{3}J-coupling restraints in protein structure determination by NMR [127,600,614].
- Determination of protein structure from chemical-shift NMR data using MD simulation [136,241].
- Structure refinement using MD simulation in four dimensions [147].
- Structure refinement using a Boltzmann-weighted conformational ensemble [199].
- Structure refinement using weak-coupling NOE distance restraining [224].
- Structure optimisation using soft-core interactions and the diffusion-equation approach [235].
- Use of time-dependent or time-averaging restraints in MD simulation [253,266,299,362,417].
- Structure refinement based on adaptive restraints [439].
- Structure refinement based on time-averaged order-parameter restraints [580,613].
- Structure refinement based on Residual Dipolar Couplings and rotational sampling [618].

9. Calculation of free energy and entropy in bio-molecular systems

- Thermodynamic cycles to compute free energy differences [63,84,132].
- Calculation of relative free energy via indirect pathways [103].
- One-step perturbation technique to calculate free energy differences [137,150,159,209,217,269,313,341,346,373,378,553,565].
- Pathway effects in free energy calculations [151,157,193,317,410,411,595].
- Decomposition of relative free energies in terms of interactions or amino acids [162,175].
- MD relative free energy calculations in four dimensions [165].
- Calculation of entropy from MD simulation [286,296,316,347,351,352,400,403,404,405,416,444,585].
- Calculation of free energy of deprotonation in solution [312].
- Method of enveloping distribution sampling (EDS) to compute relative free energies [424,448,456,466,508,519,526,535,556,557,564,571,576].
- Calculation of the free energy of polarisation [441] and quantisation [452].
- A method to compute the free enthalpy of replacing water molecules in a binding pocket [546].

10. Combining classical (MD) and quantum-mechanical treatments in bio-molecular systems

- Proton transfer using density-matrix (QM) evolution [149].
- Application of path-integral QM to water [156].
- Analysis of QM/MM simulations [182,210,221,237,246,247,267,268,293,438,523].
- Integration of the time-dependent Schrödinger equation [208].
- Non-adiabatic proton transfer in solution [239,248,274].
- Methodological aspects of QM/MM simulations [435].

11. Software development for bio-molecular simulation

- Adaptation of the implementation of MD simulation algorithms to supercomputers [33,124].
- Molecular dynamics on a multi-signal-processor system [123, 125,131].
- Groningen Molecular Simulation (GROMOS) software development [206,262,386].
- Molecular dynamics using Graphical Processor Units (GPU) [477].
- Description of the GROMOS software: architecture [525], functionalities [524,579], structure refinement [512], free energy calculation [517], analysis of trajectories [514], tutorial [610].
- Interfacing the GROMOS simulation software to quantum-chemical software [540].

12. Reviews

- Computer simulation: Methodology, applications, perspectives [99,302,402,445].
- Computer simulation: Overview of time-saving techniques [105].
- Taking account of solvation [161].
- Computer simulation of protein motion [200].
- Empirical interaction functions for molecular simulation [238,255].
- Validation of molecular dynamics simulation [244,446,605].
- Accounting for polarisation in molecular simulation [385].
- On searching, sampling and moving through conformational space [431].
- Basic ingredients and practical aspects of free energy calculations [471,578].
- Developing coarse-grained models for bio-molecular simulation [538].
- Thirty-five years of bio-molecular simulation: 1977 – 2012 (-2019) [544,607].
- Multi-resolution simulation of bio-molecular systems: methodological issues [554].
- Deriving structural information from experimentally measured data [601].
- Effects of assumptions and approximations in molecular simulation [612].

13. Protein and polypeptide folding

- Polypeptide folding [236,250,257,259,270,273,288,291,295,314,334,335,359,361,363,370,387, 392,395,399,426,434,459,463,472,478,479, 491,495,498,505,562,583,584].

14. Simulation of membranes

- MD simulation of n-dodecyl phosphate bilayers and micelles [309].
- MD simulation of lipid bilayers [315,322,357,375,382,391,394].
- MD simulation of the outer membrane protein X in a lipid bilayer and in a micelle [490].

15. Ethical issues in science

- Seven sins in the natural sciences [549].
- Pitfalls of peer review [593].
- Going for a PhD: Joys and pitfalls [598].
- Publication of research results: Use and abuse [602].
- Surfing versus drilling in fundamental research [606].

16. Proteins, peptides, DNA, sugars simulated

- bovine pancreatic trypsin inhibitor (BPTI)
  [17,20,24,25,31,55,98,129,133,139,153,168,183,198,203,615,616].
- lac repressor DNA binding domain [37,40,58,79,92,108].
- L7/L12 protein [39].
- avian pancreatic polypeptide hormone [49].
- eight-base-pair DNA [54].
- retinol-binding protein [57,59].
- insulin [60,72,107].
- cyclosporin A [64,86,97,148}.
- cyclodextrins [67,68,70,75,76,126,163,493].
- polypeptide cardiac stimulant anthopleurin-A [83].
- phospholipase A2 [85,90].
- carboxypeptidase A [88].
- bacteriophage T4 glutaredoxin [101].
- hen egg white lysozyme [118,129,153,185,195,203,277,283,303,366,483,522,539,559,613,614,617].
- subtilisin BPN' [121,138].
- antamanide [134].
- dihydrofolate reductase [137].
- flavodoxin [154].
- histidine-containing phosphocarrier protein HPr [160].
- chymotrypsin inhibitor 2 [171].
- surfactant protein C [187].
- 434 repressor DNA-binding domain [207].
- HIV-protease [221].
- antamanide [225].
- plasmodium falciparum circumsporoite surface protein [229].
- 16 base-pair DNA [252].
- alpha-lactalbumin [260,263,303,316,368,455].
- factor Xa [278,289].
- murine V_H domain [282].
- beta domain of metallothionein [285].
- estrogen receptor ligand binding domain [287].
- p-hydroxybenzoate hydroxylase [293].
- alpha-helical surfactant-associated polypeptide C [301].

- llama antibody heavy-chain variable domain [303].
- fatty acid binding protein [303,323,325].
- ubiquitin [305,425,469].
- photoactive yellow protein [336].
- quercetinase [364].
- azurin [372,530].
- bee venom mellitin [391].
- arc repressor protein [408].
- cyclophilin [414].
- cytochrome c [415].
- human interleukin-4 [440,604].
- ccß-Met amyloid [442].
- ASC and NALP1 pyrin domains [443].
- ankyrin repeat protein [454].
- HET-s(218-289) prion [460,596].
- TRP-cage mini protein TC5b [467].
- GFP chromophore [482].
- outer membrane protein X [490].
- plasmepsin II [503].
- phenylethanolamine N-methyltransferase [508].
- french bean plastocyanin [531].
- p53 core domain {541].
- chorismate mutase [542].
- barley and maize lipid transfer protein [550].
- AppA BLUF domain [558].
- isochorismate pyruvate lyase [560].
- protein G [563].
- bacteriophage lambda lysozyme [587].
- protein hGH [603].

17. Liquids, solvents simulated

- water [18,202,324,338,340,365,465,497,579,581].
- chloroform [171,487,527].
- dimethyl sulfoxide [189,349,527,577].
- carbon tetrachloride [223,496].
- methanol [276,406,527].
- urea [348,586].
- acetonitrile [393].
- ethylene glycol [432].
- dimethyl sulfone [516].
- acetone [597].