



The GLOBE-Consortium

Erasmus Computing Grid



The Erasmus Computing Grid Building a Super-Computer at Erasmus MC for *Free*

by

Rob de Graaf, Remko Kleinjan, Redmar van Leeuwarden, Sander van Vliet

Bert Eussen, Michael Moorhouse & Tobias A. Knoch

Clinical Genetics, Virology, Cell Biology & Genetics

Erasmus MC, Rotterdam, The Netherlands

Contact: globe@erasmusmc.nl and <http://www.erasmusmc.nl/globe-consortium>

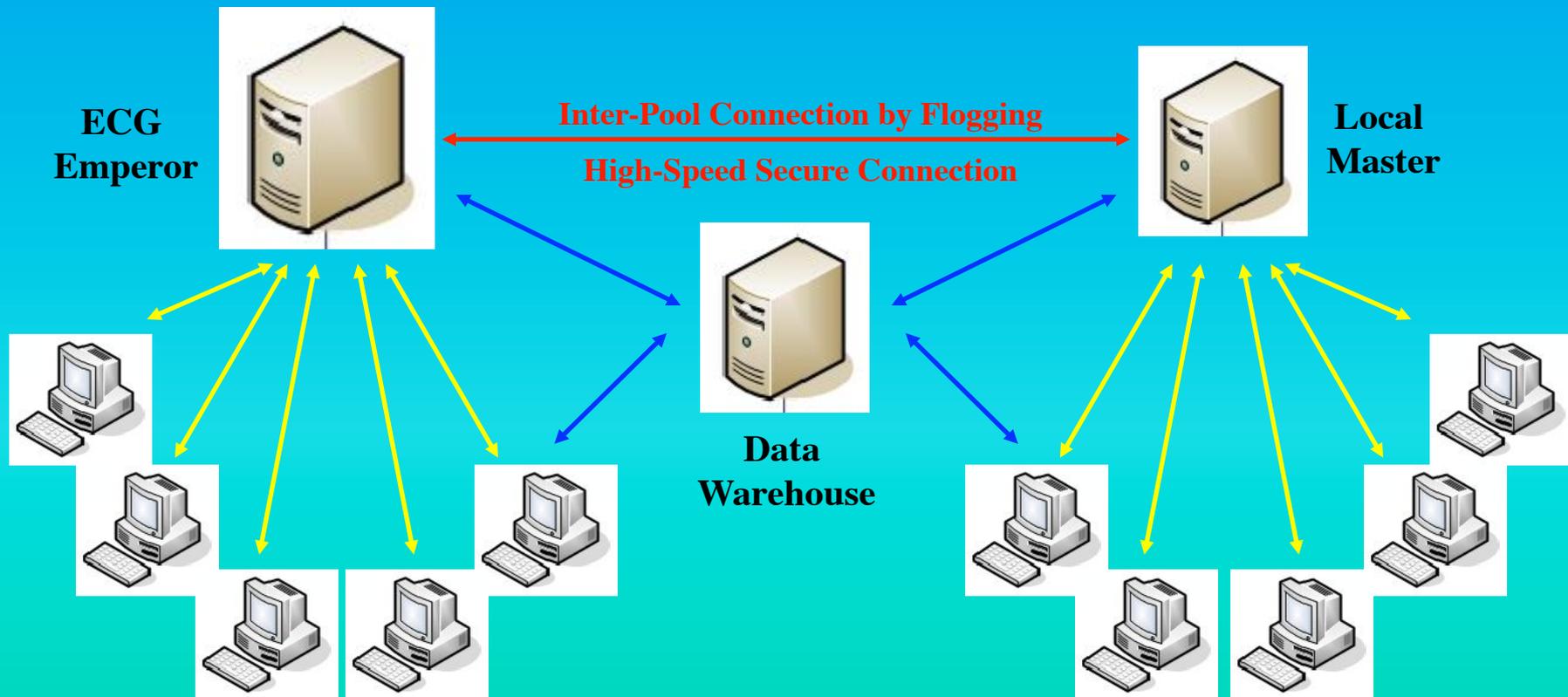
ECG Basic Grid Structure

The ECG consists of the computer pools the Erasmus MC and the Hogeschool Rotterdam. The client computers are controlled by the general ECG Emperor of the grid at EMC and a local master at HR. "Condor" is used as middleware since it is very well established and open-source.

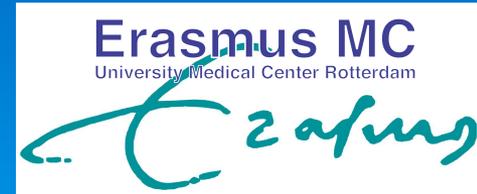


~9000 CPUs or ~18000 vHosts

~3500 CPUs or ~7000 vHosts

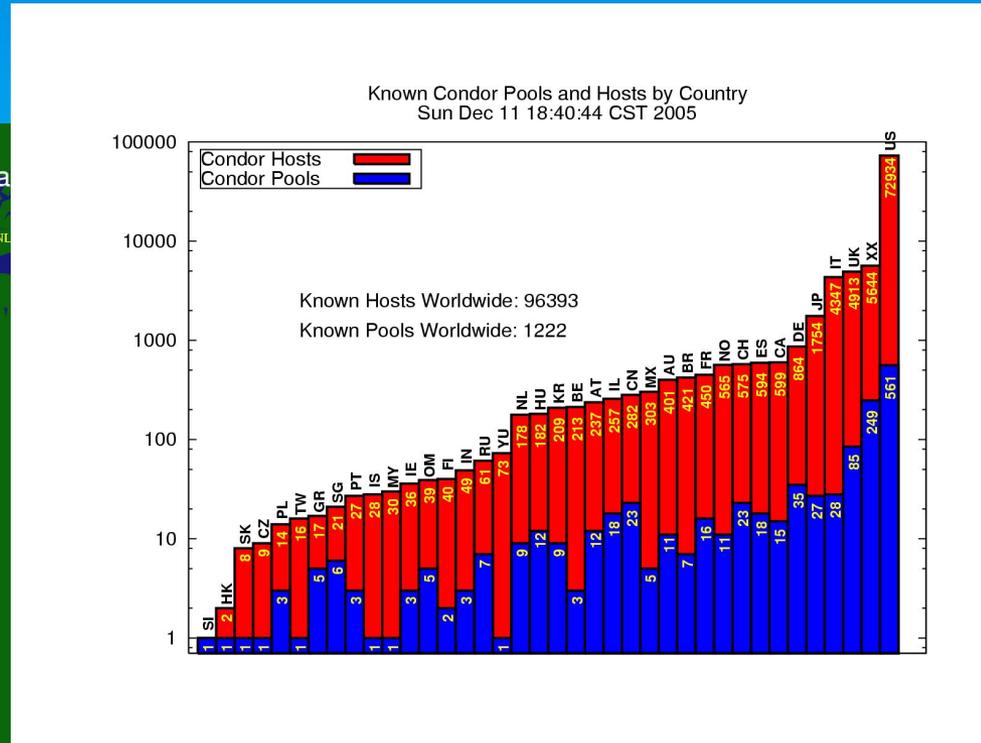
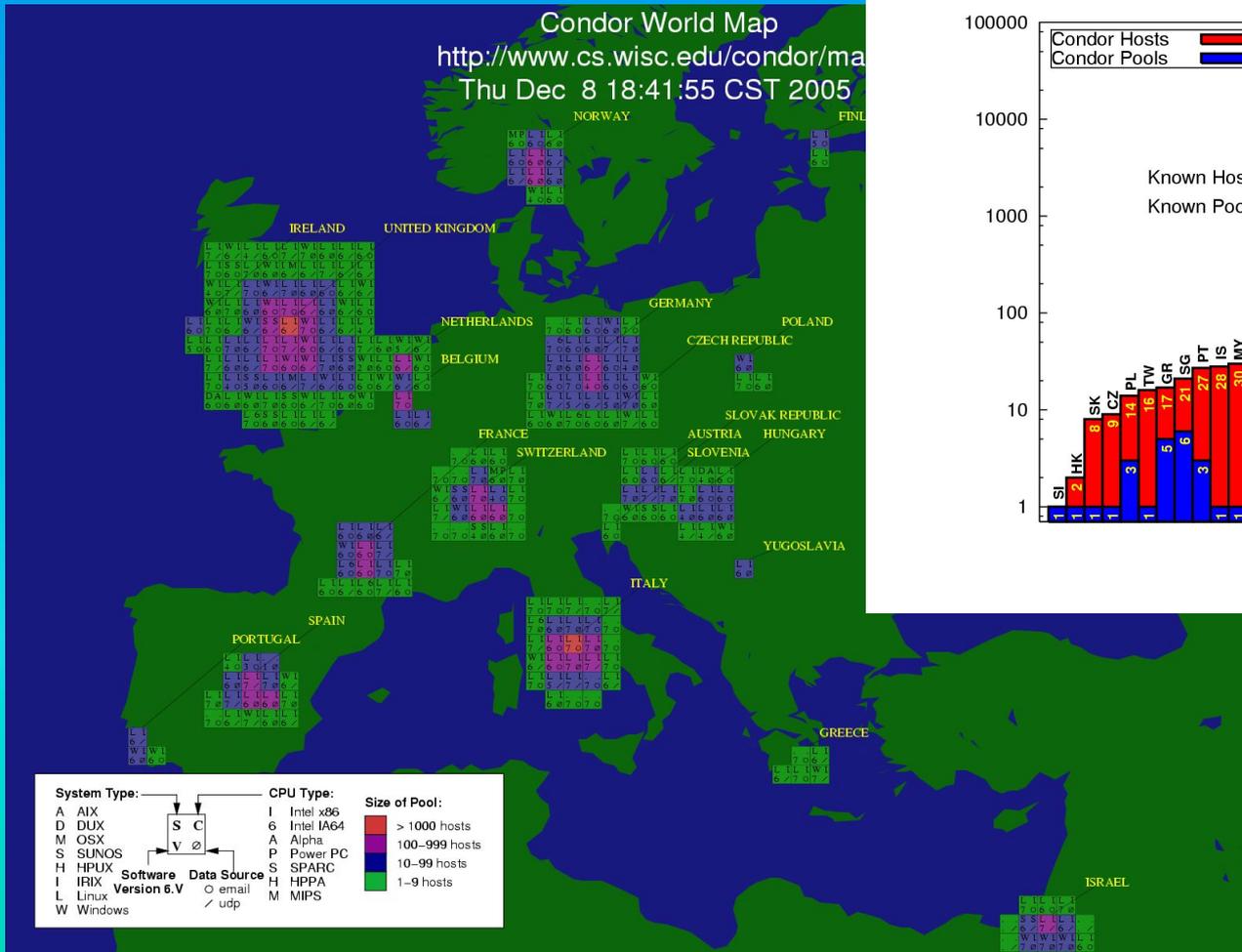


World-Map of Condor Grids



Condor is used as the standard for batch systems on many real parallel super-computers as well as in many distributed trivial parallel computing grids. It is running in very diverse environments of the highest security levels as e.g. governmental or industry R&D.

With a potential capacity of ~20.000 Gflops the ECG could become one the 20 biggest grids!



Based on pool operator reports only!

Installation and Security

For installation, Condor is installed administratively via a secure login from the ECG management site using the corresponding installers.

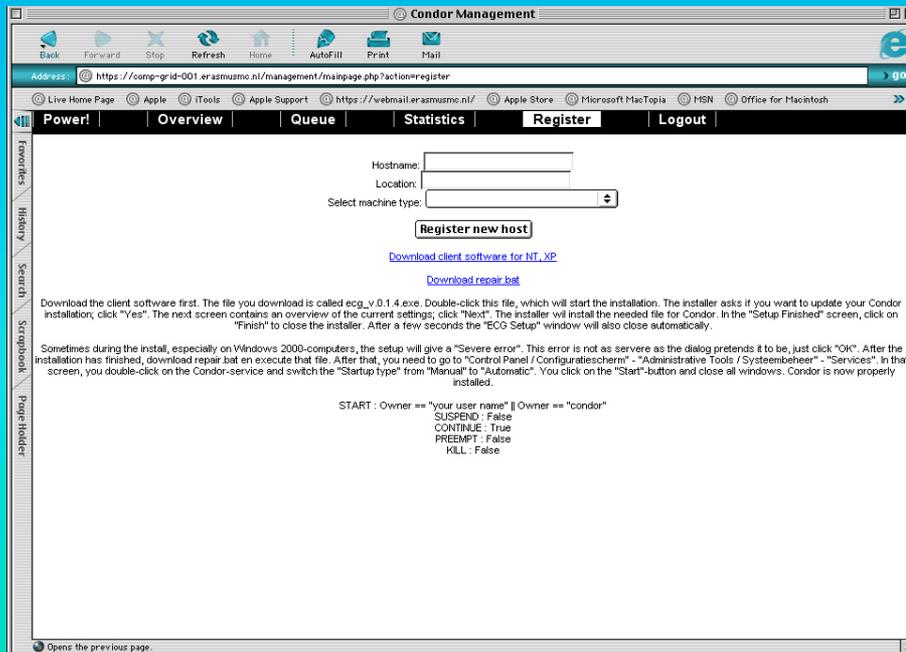
Condor is an established middleware with no known risks: Condor is running as a guest, no data can be accessed in any form, and nothing can be changed on the local client computer!



Installation

2 Minutes per computer using the ECG management system

- ❖ software install
- ❖ registration
- ❖ general maintenance



Security

The ECG is NO Risk to the client computer or EMC/HR

- ❖ runs as a *guest*
- ❖ data connection to master is *secure*
- ❖ no local data are visible to condor
- ❖ the local system *cannot* be changed
- ❖ application executables are *certified*
- ❖ input data is *certified* by ECG
- ❖ local user *always* has usage priority
- ❖ runs *only* if vhosts are available
- ❖ jobs can be stopped *always* automatically
- ❖ ECG can be used as a security monitoring system (e.g. power outage or flooding)
- ❖ **PRIVACY RULES ARE APPLIED AND GUARANTIED!!!**

ECG - Management

To maintain the ECG a data base with installed and registered hosts was created. It allows to track the status of the local clients and gives global statistical data about performance. A job-submission and accounting system is currently implemented.

Usage of the grid is through the GLOBE-Consortium in a secure manner only!



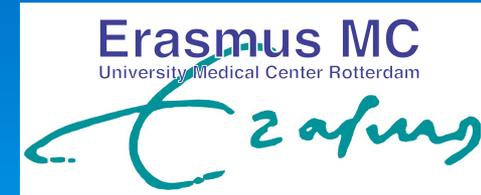
The screenshot shows the Condor Management web interface. The browser window title is "Condor Management". The address bar shows the URL: <https://comp-grid-001.erasmusmc.nl/management/mainpage.php?action=status&display=table>. The page contains a table of host statistics and a central speedometer graphic.

Host	IP	MFlops	MB	...	Time	...
vm1@TigerLion	10.98.4.7	695.16	511 MB	0	2005-11-07 13:20:19.777098	[x][i]
vm2@TigerLion	10.98.4.7	695.16	511 MB	0	2005-11-07 13:20:19.977908	[x][i]
vm3@TigerLion					11-07 13:20:20.185658	[x][i]
vm4@TigerLion					11-07 13:20:20.389709	[x][i]
vm1@bioinf-mir.erasmusmc.nl					11-07 13:20:01.606706	[x][i]
vm2@bioinf-mir.erasmusmc.nl					11-07 13:20:01.801927	[x][i]
vm3@bioinf-mir.erasmusmc.nl					11-07 13:20:01.996655	[x][i]
vm4@bioinf-mir.erasmusmc.nl					11-07 13:20:02.194894	[x][i]
vm1@cbg-grid.gen.fgg.eur.nl					11-07 13:20:02.404949	[x][i]
vm2@cbg-grid.gen.fgg.eur.nl					11-07 13:20:02.60134	[x][i]
vm1@cbg3.erasmusmc.nl					11-07 13:20:02.887505	[x][i]
vm2@cbg3.erasmusmc.nl					11-07 13:20:03.086038	[x][i]
vm3@cbg3.erasmusmc.nl					11-07 13:20:03.282584	[x][i]
vm4@cbg3.erasmusmc.nl					11-07 13:20:03.481282	[x][i]
ch1-42402679					11-07 13:20:05.17493	[x][i]
dell1032221204					11-07 13:20:05.369733	[x][i]
dell103233481	10.98.25.63	712.76	509 MB	0	2005-11-07 13:20:05.566907	[x][i]

The central speedometer graphic is labeled "GigaFlops/cluster" and shows a needle pointing to approximately 60. A red star is overlaid on the speedometer with the text "10001 hosts" and a "Login" button above it.

Opportunities

The GLOBE-Consortium has started to establish successfully a Super-Computer at Erasmus MC!

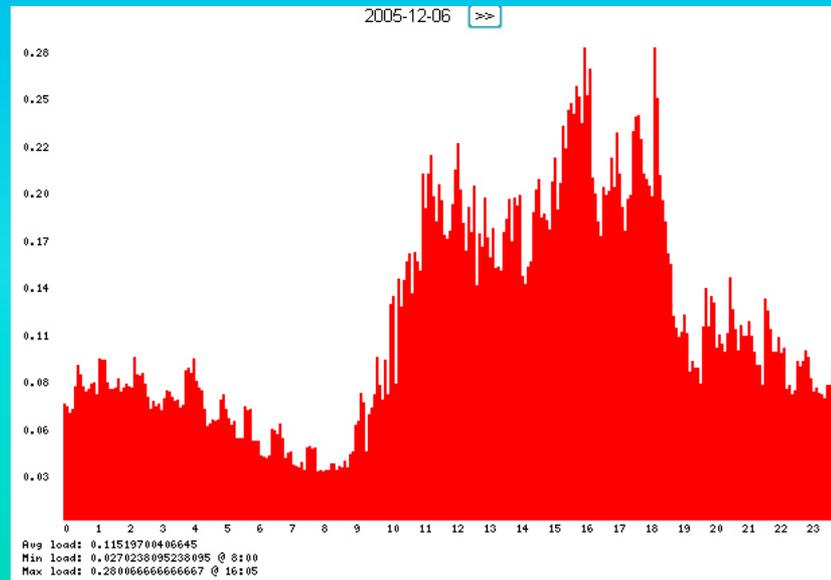


The Erasmus Computing Grid:

The Erasmus Computing Grid greatly advances the computing capabilities of the Erasmus Mc, e.g. for:

- ❖ genomic and proteomic analysis
- ❖ epidemiology
- ❖ clinical image analysis, e.g. Applied Molecular Imaging (AMI)

The Erasmus Computing Grid has also great potential for commercialization!



The GLOBE-Consortium: The Erasmus Computing Grid

–

Building a Super-Computer at Erasmus MC for FREE

Knoch, T. A.

Bridge Meeting, Erasmus Medical Center, Erasmus University of Rotterdam, Rotterdam, The Netherlands, September, 2005.

Abstract

To meet the enormous computational needs of live-science research as well as clinical diagnostics and treatment the Hogeschool Rotterdam and the Erasmus Medical Center are currently setting up one of the largest desktop computing grids in the world – The Erasmus Computing Grid. Currently 3 Tera flops are operational and in early production, installation up to the today available maximum capacity of 20 Tera flops in both institutions is planned and partly underway. Thus the Erasmus Computing Grid transforms the existing and sustained huge computer capacity available into usable form via a reliable and secure installing and management system, so that the academic and industrial opportunities depending on such huge computing capacities can be realized for the benefit of society.

Corresponding author email contact: TA.Knoch@taknoch.org

Keywords:

Genome, genomics, genome organization, genome architecture, structural sequencing, architectural sequencing, systems genomics, coevolution, holistic genetics, genome mechanics, genome function, genetics, gene regulation, replication, transcription, repair, homologous recombination, simultaneous co-transfection, cell division, mitosis, metaphase, interphase, cell nucleus, nuclear structure, nuclear organization, chromatin density distribution, nuclear morphology, chromosome territories, subchromosomal domains, chromatin loop aggregates, chromatin rosettes, chromatin loops, chromatin fibre, chromatin density, persistence length, spatial distance measurement, histones, H1.0, H2A, H2B, H3, H4, mH2A1.2, DNA sequence, complete sequenced genomes, molecular transport, obstructed diffusion, anomalous diffusion, percolation, long-range correlations, fractal analysis, scaling analysis, exact yard-stick dimension, box-counting dimension, lacunarity dimension, local nuclear dimension, nuclear diffuseness, parallel super computing, grid computing, volunteer computing, Brownian Dynamics, Monte Carlo, fluorescence in situ hybridization, confocal laser scanning microscopy, fluorescence correlation spectroscopy, super resolution microscopy, spatial precision distance microscopy, auto-fluorescent proteins, CFP, GFP, YFP, DsRed, fusion protein, in vivo labelling, information browser, visual data base access, holistic viewing system, integrative data management, extreme visualization, three-dimensional virtual environment, virtual paper tool.

Literature References

- Knoch, T. A.** Dreidimensionale Organisation von Chromosomen-Domänen in Simulation und Experiment. (Three-dimensional organization of chromosome domains in simulation and experiment.) *Diploma Thesis*, Faculty for Physics and Astronomy, Ruperto-Carola University, Heidelberg, Germany, 1998, and TAK Press, Tobias A. Knoch, Mannheim, Germany, ISBN 3-00-010685-5 and ISBN 978-3-00-010685-9 (soft cover, 2nd ed.), ISBN 3-00-035857-9 and ISBN 978-3-00-0358857-0 (hard cover, 2nd ed.), ISBN 3-00-035858-7, and ISBN 978-3-00-035858-6 (DVD, 2nd ed.), 1998.
- Knoch, T. A., Münkkel, C. & Langowski, J.** Three-dimensional organization of chromosome territories and the human cell nucleus - about the structure of a self replicating nano fabrication site. *Foresight Institute - Article Archive*, Foresight Institute, Palo Alto, CA, USA, <http://www.foresight.org>, 1- 6, 1998.
- Knoch, T. A., Münkkel, C. & Langowski, J.** Three-Dimensional Organization of Chromosome Territories and the Human Interphase Nucleus. *High Performance Scientific Supercomputing*, editor Wilfried Juling, Scientific Supercomputing Center (SSC) Karlsruhe, University of Karlsruhe (TH), 27- 29, 1999.
- Knoch, T. A., Münkkel, C. & Langowski, J.** Three-dimensional organization of chromosome territories in the human interphase nucleus. *High Performance Computing in Science and Engineering 1999*, editors Krause, E. & Jäger, W., High-Performance Computing Center (HLRS) Stuttgart, University of Stuttgart, Springer Berlin-Heidelberg-New York, ISBN 3-540-66504-8, 229-238, 2000.
- Bestvater, F., **Knoch, T. A.**, Langowski, J. & Spiess, E. GFP-Walking: Artificial construct conversions caused by simultaneous cotransfection. *BioTechniques* 32(4), 844-854, 2002.
- Knoch, T. A. (editor)**, Backes, M., Baumgärtner, V., Eysel, G., Fehrenbach, H., Göker, M., Hampl, J., Hampl, U., Hartmann, D., Hitzelberger, H., Nambena, J., Rehberg, U., Schmidt, S., Weber, A., & Weidemann, T. Humanökologische Perspektiven Wechsel - Festschrift zu Ehren des 70. Geburtstags von Prof. Dr. Kurt Egger. Human Ecology Working Group, Ruperto-Carola University of Heidelberg, Heidelberg, Germany, 2002.
- Knoch, T. A.** Approaching the three-dimensional organization of the human genome: structural-, scaling- and dynamic properties in the simulation of interphase chromosomes and cell nuclei, long- range correlations in complete genomes, *in vivo* quantification of the chromatin distribution, construct conversions in simultaneous co-transfections. *Dissertation*, Ruperto-Carola University, Heidelberg, Germany, and TAK†Press, Tobias A. Knoch, Mannheim, Germany, ISBN 3-00-009959-X and ISBN 978-3-00-009959-5 (soft cover, 3rd ed.), ISBN 3-00-009960-3 and ISBN 978-3-00-009960-1 (hard cover, 3rd ed.), ISBN 3-00-035856-9 and ISBN 978-3-00-010685-9 (DVD, 3rd ed.) 2002.
- Knoch, T. A.** Towards a holistic understanding of the human genome by determination and integration of its sequential and three-dimensional organization. *High Performance Computing in Science and Engineering 2003*, editors Krause, E., Jäger, W. & Resch, M., High-Performance Computing Center (HLRS) Stuttgart, University of Stuttgart, Springer Berlin-Heidelberg-New York, ISBN 3- 540-40850-9, 421-440, 2003.
- Wachsmuth, M., Weidemann, T., Müller, G., Urs W. Hoffmann-Rohrer, **Knoch, T. A.**, Waldeck, W. & Langowski, J. Analyzing intracellular binding and diffusion with continuous fluorescence photobleaching. *Biophys. J.* 84(5), 3353-3363, 2003.
- Weidemann, T., Wachsmuth, M., **Knoch, T. A.**, Müller, G., Waldeck, W. & Langowski, J. Counting nucleosomes in living cells with a combination of fluorescence correlation spectroscopy and confocal imaging. *J. Mol. Biol.* 334(2), 229-240, 2003.
- Fejes Tóth, K., **Knoch, T. A.**, Wachsmuth, M., Frank-Stöhr, M., Stöhr, M., Bacher, C. P., Müller, G. & Rippe, K. Trichostatin A induced histone acetylation causes decondensation of interphase chromatin. *J. Cell Science* 117, 4277-4287, 2004.
- Ermler, S., Kronic, D., **Knoch, T. A.**, Moshir, S., Mai, S., Greulich-Bode, K. M. & Boukamp, P. Cell cycle-dependent 3D distribution of telomeres and telomere repeat-binding factor 2 (TRF2) in HaCaT and HaCaT-myc cells. *Europ. J. Cell Biol.* 83(11-12), 681-690, 2004.

- Kost, C., Gama de Oliveira, E., **Knoch, T. A.** & Wirth, R. Spatio-temporal permanence and plasticity of foraging trails in young and mature leaf-cutting ant colonies (*Atta spp.*). *J. Trop. Ecol.* 21(6), 677- 688, 2005.
- Winnefeld, M., Grewenig, A., Schnölzer, M., Spring, H., **Knoch, T. A.**, Gan, E. C., Rommelaere, J. & Czipluch, C. Human SGT interacts with BAG-6/Bat-3/Scythe and cells with reduced levels of either protein display persistence of few misaligned chromosomes and mitotic arrest. *Exp. Cell Res.* 312, 2500-2514, 2006.