

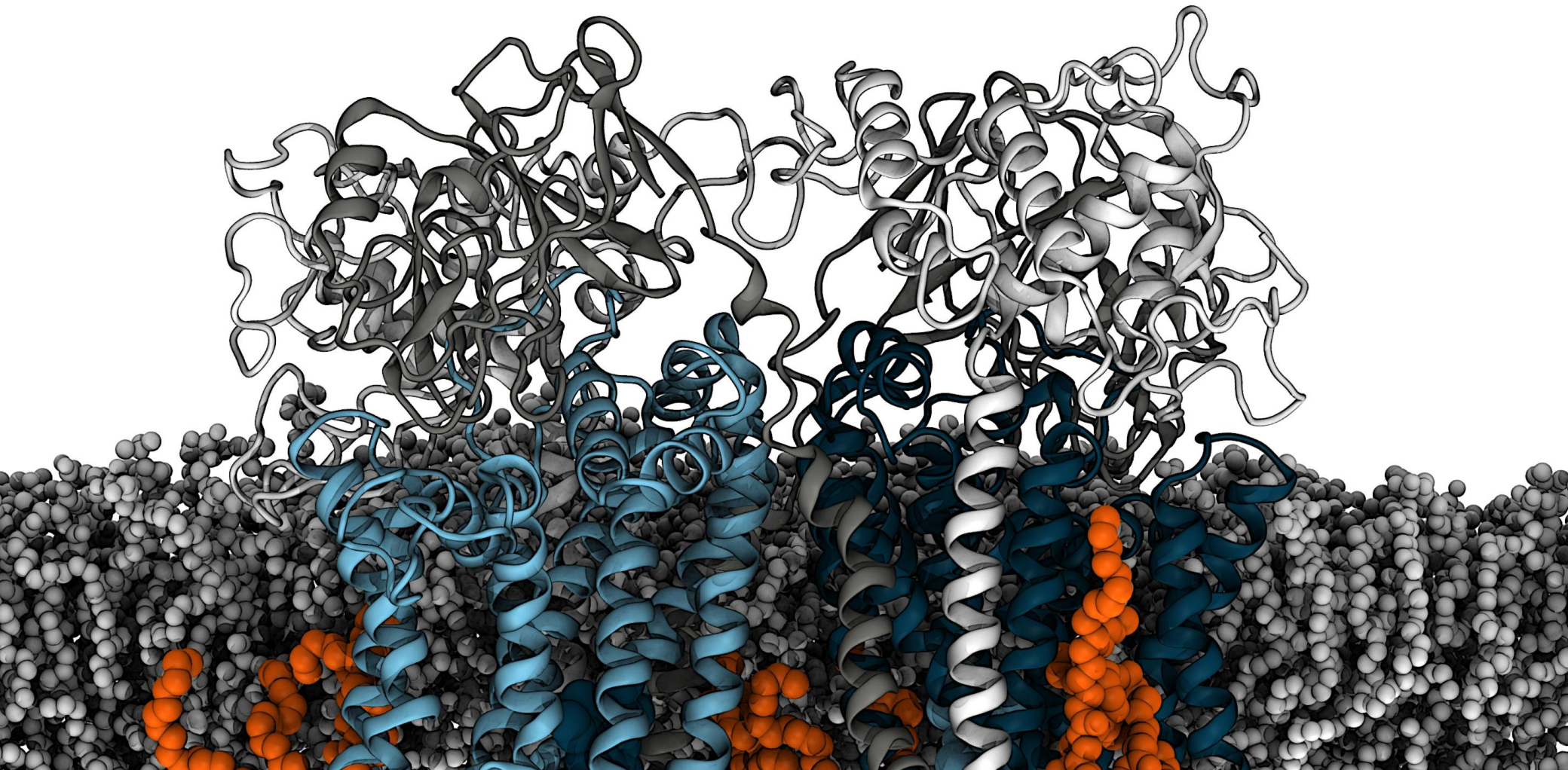
Tekijyys - Authorship

Ilpo Vattulainen

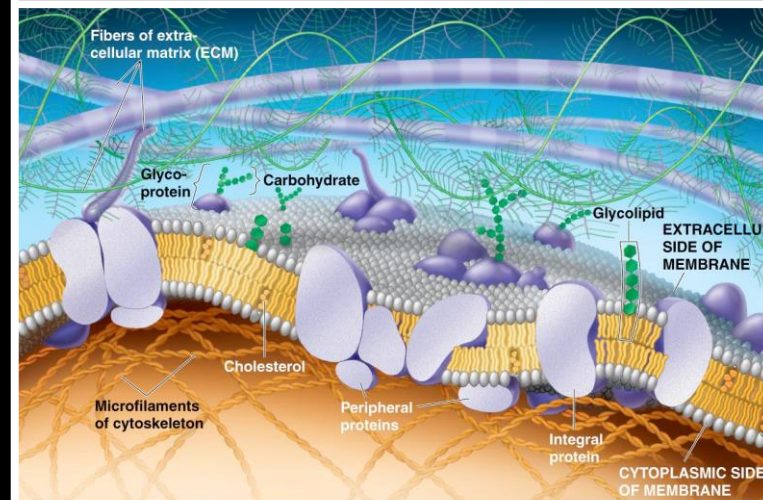
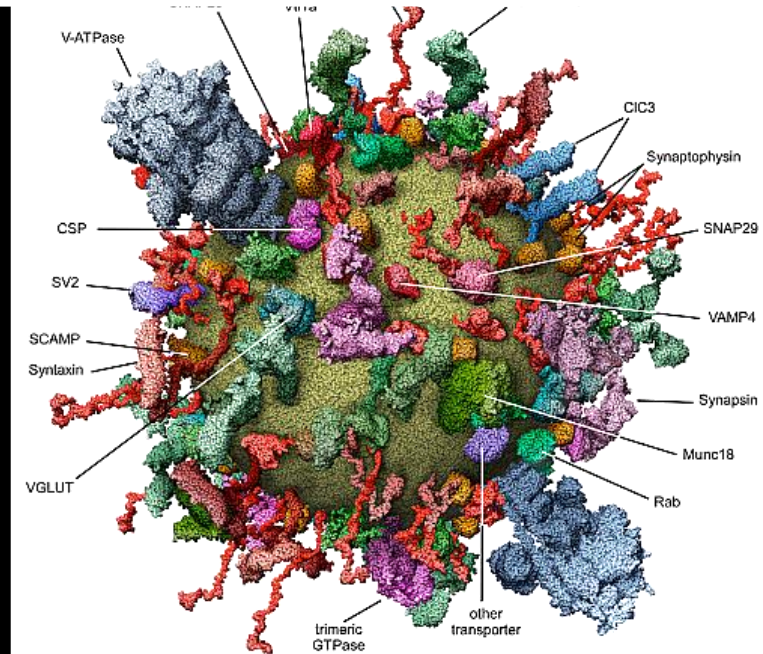
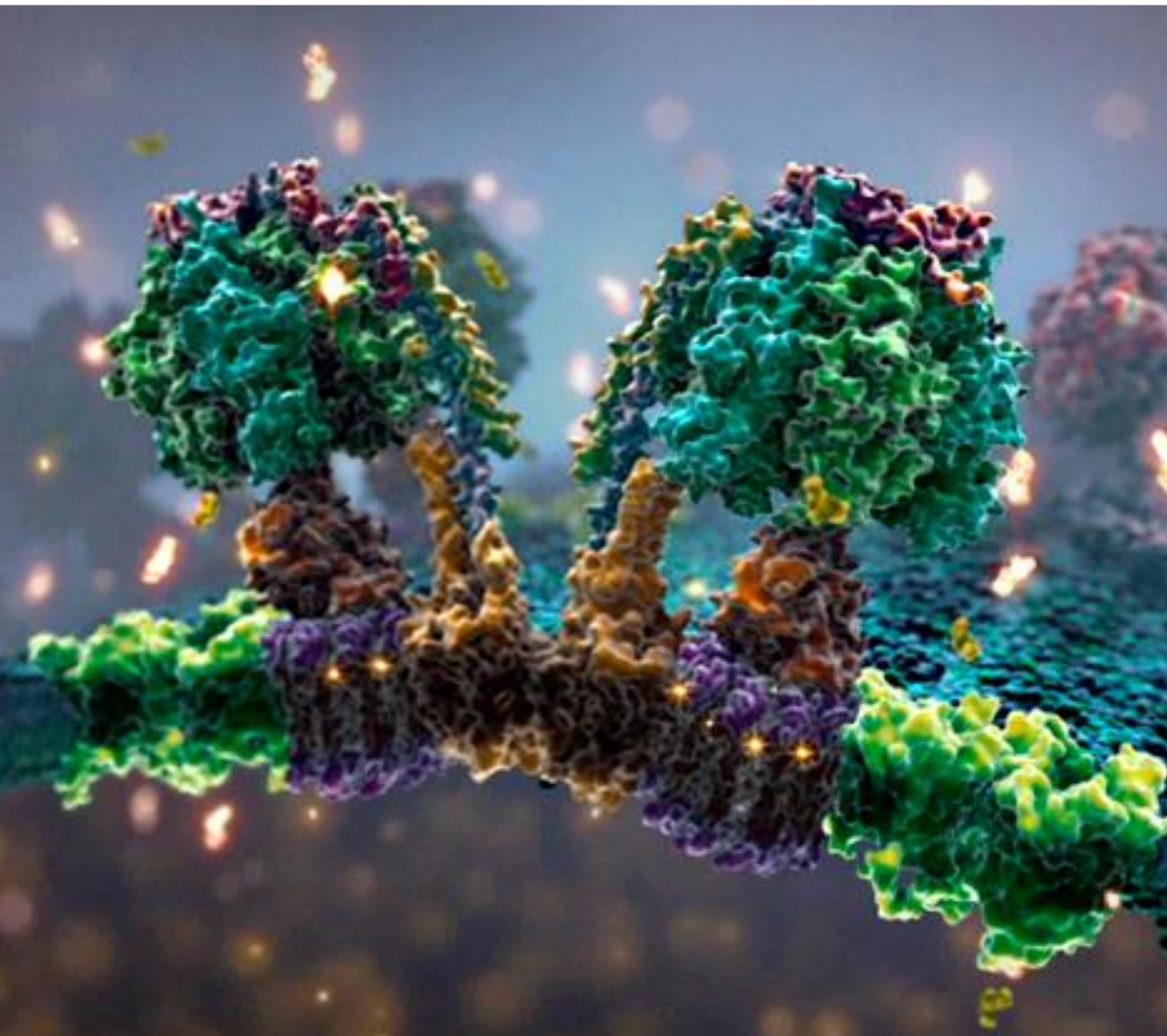
Tampere Univ of Tech & Univ Helsinki

Center of Excellence in Biomembrane Research

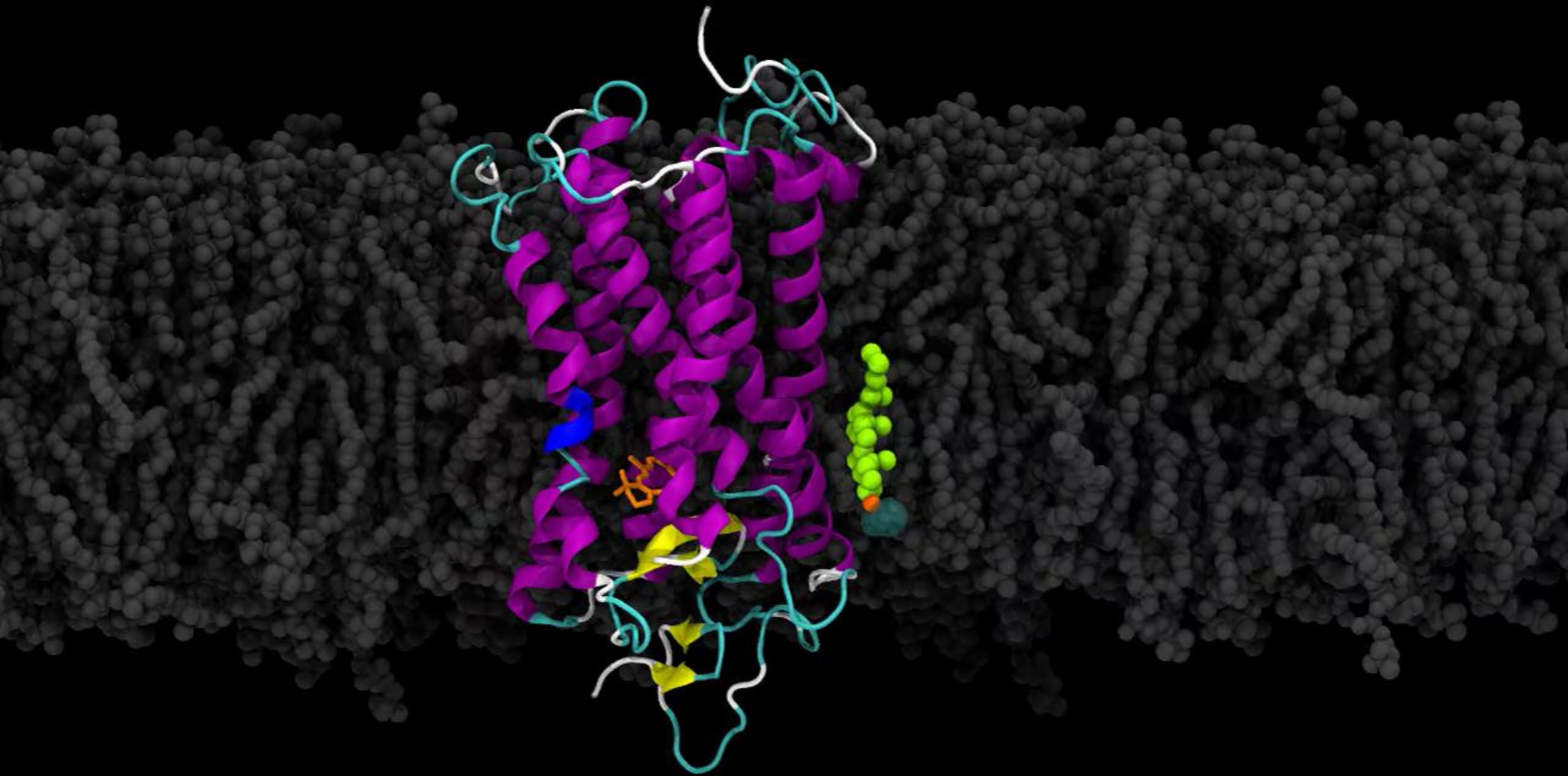
ERC Advanced Grant (2012-2017)



YLEINEN MOTIVAATIO: YMMÄRTÄÄ SOLUJEN POSTIN VÄLITYS - ATOMITASOLLA



LIPIDIEN (RASVOJEN) DYNAMIIKKA SOLUKALVOISSA

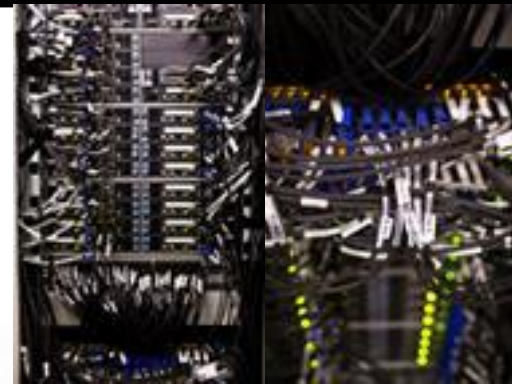


RYHMÄ: NOIN 35 + 35 IHMISTÄ



Biological Physics
Prof Ilpo Vattulainen
~35 people
ERC Advanced Grant

Biophysics
Academy Research
Fellow
Tomasz Rog



Protein Simulations
Prof Pavel Jungwirth
(Prague)
FiDiPro
~20 people



Stat Mech
Prof Ralf Metzler
(Potsdam)
FiDiPro
~15 people



MATEMATIKAN TUTKIJAN ARKEA

Proc. Natl. Acad. Sci. USA
Vol. 95, pp. 98–101, January 1998
Computer Sciences

***P/*NP, and the quantum field computer**

MICHAEL H. FREEDMAN

Microsoft Research 9N, 1 Microsoft Way, Redmond, WA 98052

Contributed by Michael H. Freedman

ABSTRACT The central problem in computer science is the conjecture that two complexity classes, P (polynomial time) and NP (nondeterministic polynomial time—roughly those decision problems for which a proposed solution can be checked in polynomial time), are distinct in the standard Turing model of computation: $P \neq NP$. As a generality, we propose that each physical theory supports computational models whose power is limited by the physical theory. It is well known that classical physics supports a multitude of implementations of the Turing machine. Non-Abelian topological

and a tape. The head is capable of being in one of a finite number of “internal states” $\{q_i\}$ and can read and overwrite a symbol $\in \{S_j\}$ from a finite set of symbols and then shift one block left or right along the tape. It contains a finite internal program that directs its operations.

Consider a problem Q , with a yes/no answer, for which infinitely many instances exist, for example, the satisfiability of Boolean formulae. One asks: what is the fastest possible running time as a function of the size of the instance which a fixed program might achieve in correctly answering all of the

RYHMÄN SISÄINEN YHTEISTYÖ

Protein crowding in lipid bilayers gives rise to non-Gaussian anomalous lateral diffusion of phospholipids and proteins

Jae-Hyung Jeon,^{1,2} Matti Javanainen,² Hector Martinez-Seara,² Ralf Metzler,^{3,2} and Ilpo Vattulainen^{2,4}

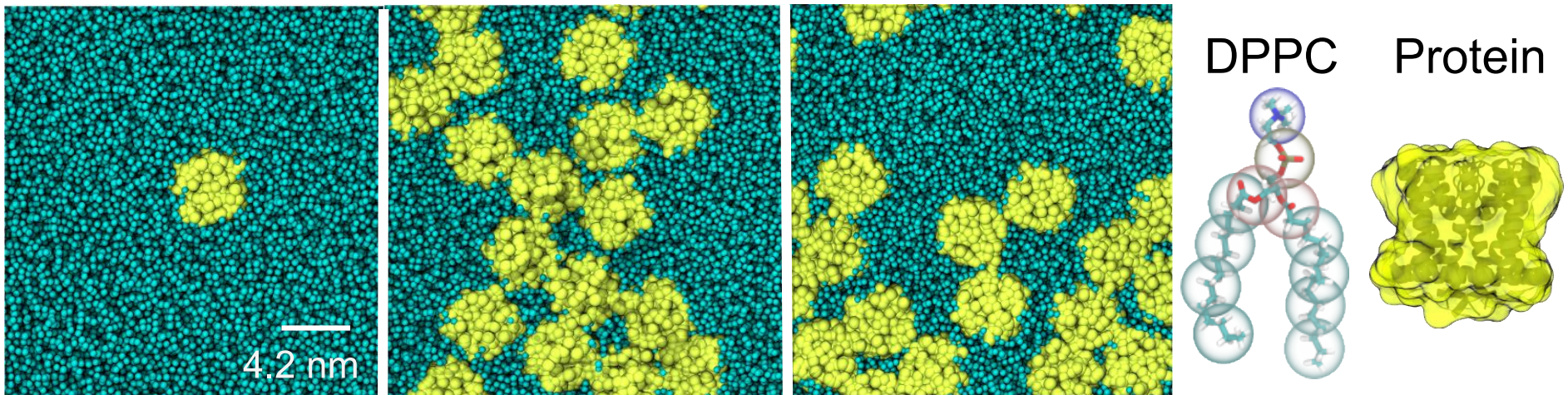
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²*Department of Physics, Tampere University of Technology, FI-33101 Tampere, Finland*

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⁴*Memphys – Center for Biomembrane Physics, University of Southern Denmark, DK-5230, Odense, Denmark*

(Dated: August 31, 2015)



RYHMIEN VÄLINEN YHTEISTYÖ EUROOPASSA

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Original Contribution

Cholesterol under oxidative stress—How lipid membranes sense oxidation as cholesterol is being replaced by oxysterols



Waldemar Kulig^{a,*}, Agnieszka Olżyńska^b, Piotr Jurkiewicz^{b,*}, Anu M. Kantola^c,
Sanna Komulainen^c, Moutusi Manna^a, Mohsen Pourmoussa^a, Mario Vazdar^{a,d},
Lukasz Cwiklik^{b,e,*}, Tomasz Rog^a, George Khelashvili^f, Daniel Harries^g,
Ville-Veikko Telkki^c, Martin Hof^b, Ilpo Vattulainen^{a,h}, Pavel Jungwirth^{e,a}

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^h MEMPHYS—Center for Biomembrane Physics, University of Southern Denmark, Odense, Denmark

Sec14-nodulin proteins and the patterning of phosphoinositide landmarks for developmental control of membrane morphogenesis

Ratna Ghosh^{a,*}, Marília K. F. de Campos^{b,*}, Jin Huang^a, Seong K. Huh^a, Adam Orłowski^c, Yuan Yang^d, Ashutosh Tripathi^a, Aaron Nile^a, Hsin-Chieh Lee^b, Marek Dynowski^e, Helen Schäfer^b, Tomasz Róg^c, Marta G. Lete^f, Hasna Ahyayauch^{f,g}, Alicia Alonso^f, Ilpo Vattulainen^{c,h}, Tatyana I. Igumenova^d, Gabriel Schaaf^b, and Vytas A. Bankaitis^{a,d,i}

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EETTISET SÄÄNNÖT - LUONNONTIETEET

"authorship should be limited to those who have contributed substantially to the work"

EETTISET SÄÄNNÖT – LÄÄKE- JA BIOLOGISET TIETEET

"The author must have:

- ***Contributed substantially to the conception and design of the study, the acquisition of data, or the analysis and interpretation***
 - ***Drafted or provided critical revision of the article***
 - ***Provided final approval of the version to publish***
- Acquisition of funding, or general supervision of the research group alone does **not** constitute authorship."***

(1) TEKIJÖIDEN VALINTAA KÄYTÄNNÖSSÄ OMASSA YKSIKÖSSÄMME

Protein crowding in lipid bilayers gives rise to non-Gaussian anomalous lateral diffusion of phospholipids and proteins

Jae-Hyung Jeon,^{1,2} Matti Javanainen,² Hector Martinez-Seara,² Ralf Metzler,^{3,2} and Ilpo Vattulainen^{2,4}

Merkittävä kontribuutio?

- **Idea, implementoinnin toteutuksen suunnittelu, toteutus osakokonaisuus kerrallaan, analyysi, tulkinta, kirjoitus, jne.**
- **Toteutus & analyysi vaatii usein monen ihmisen kontribuutiota – muuten projektilla ei ole onnistumisen mahdollisuutta järkevässä ajassa**
- **Tulkinta erilainen juniorille ja seniorille: mitä kokeneempi, sitä enemmän vaaditaan**
- **Kyse ei ole tehdyn työn määrästä tai käytetystä ajasta: 15 min keskustelu saattaa olla tärkeämpi kuin 1 vuoden suorittava työ**
- **Palkan maksaminen voi olla tieteellinen kontribuutio, jos sen hankkiminen on perustunut projektin tieteellisen idean tuottamiseen**
- **Oikeus todeta, että oma kontribuutio ei ole riittävä**

(1) TEKIJÖIDEN VALINTAA KÄYTÄNNÖSSÄ OMASSA YKSIKÖSSÄMME

Protein crowding in lipid bilayers gives rise to non-Gaussian anomalous lateral diffusion of phospholipids and proteins

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Tekijöiden valinta

- Tekijöitä ei valita projektin alussa – valinta vasta artikkelia kirjoitettaessa
- Tutkijalla oikeus ehdottaa, että kuuluu tekijöiden listaan
- Projektin jäsenillä velvollisuus ehdottaa, jos tekijäluettelosta puuttuu joku tieteellisen kontribuution omaava
- Valinta tekijäksi osin yhteisöllinen päätös siitä, onko *tieteellinen kontribuutio* ollut merkittävä – lopullinen päätös projektin vetäjällä
- Monen ryhmän yhteistyössä tekijöiden valinta perustuu luottamukseen
- Usean projektin jatkumossa tekijyyttä voi tarkastella artikkeliportfolion kannalta kokonaisuutena
- Intohimoristiriita: Ensimmäisiä (ja viimeisiä) tekijöitä voi olla useampi

Kiitos

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- Academy of Finland
- ERC
- EU FP7
- Bioindustry
- Tekes
- Finnish Foundations
- CSC & PRACE (Tier-0, Tier-1)

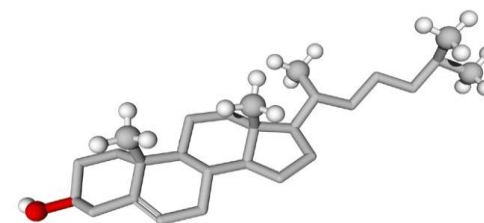


Collaborators (experiments, examples):

Elina Ikonen (Biomedicum, Hki)
Kai Simons (MPI Dresden)
Ünal Coskun (Dresden)
Christian Eggeling (Göttingen)
Petri Kovanen (Wihuri, Hki)
Peter Westh (Roskilde)
Juha Holopainen (HUS, Hki)
Susanne Wiedmer (Hki)

Collaborators (theory, examples):

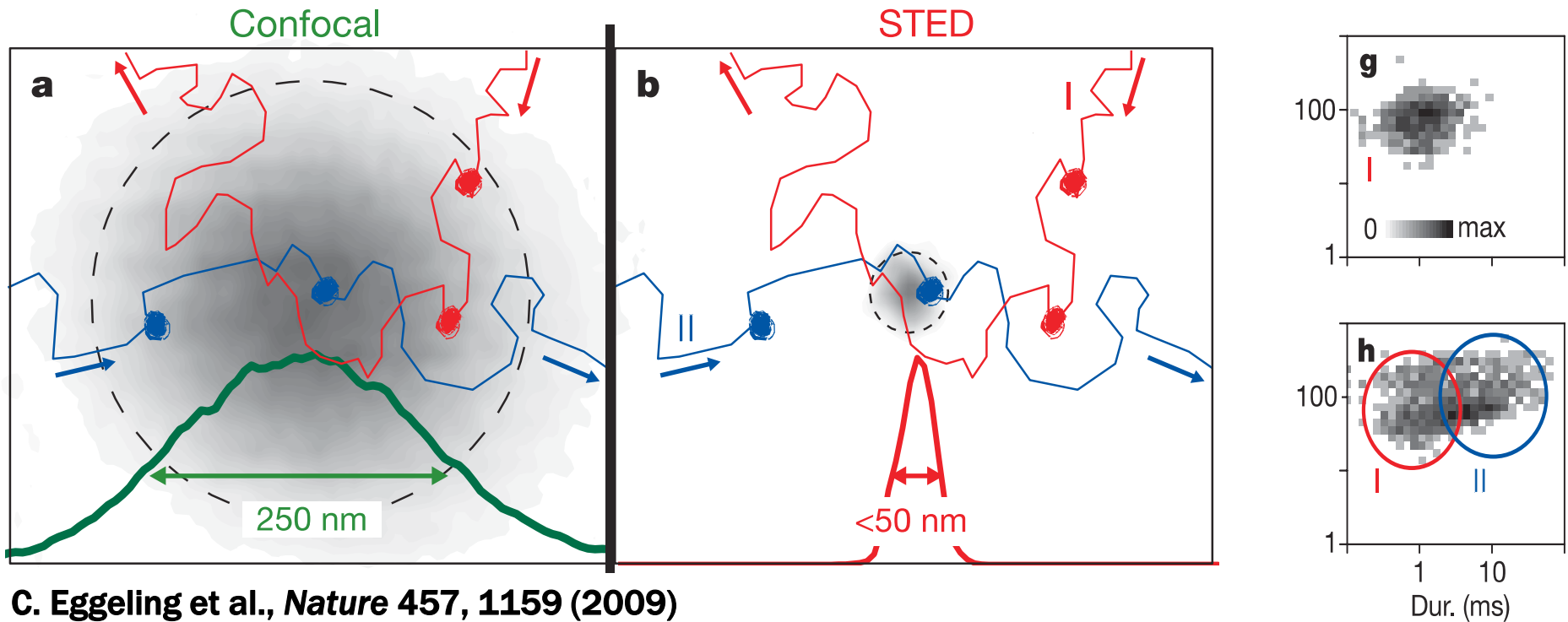
Mikko Karttunen (Waterloo)
Roland Faller (UC Davis)
Tapio Ala-Nissilä (Aalto)
Matej Oresic et al. (VTT)
Erik Lindahl (Stockholm)
Alex Bunker (Viikki/Drug Design)
SJ Marrink (Groningen)
AA Gurtovenko (St. Petersburg)



Networks:

NordForsk, Nordita, Graduate Schools, etc.

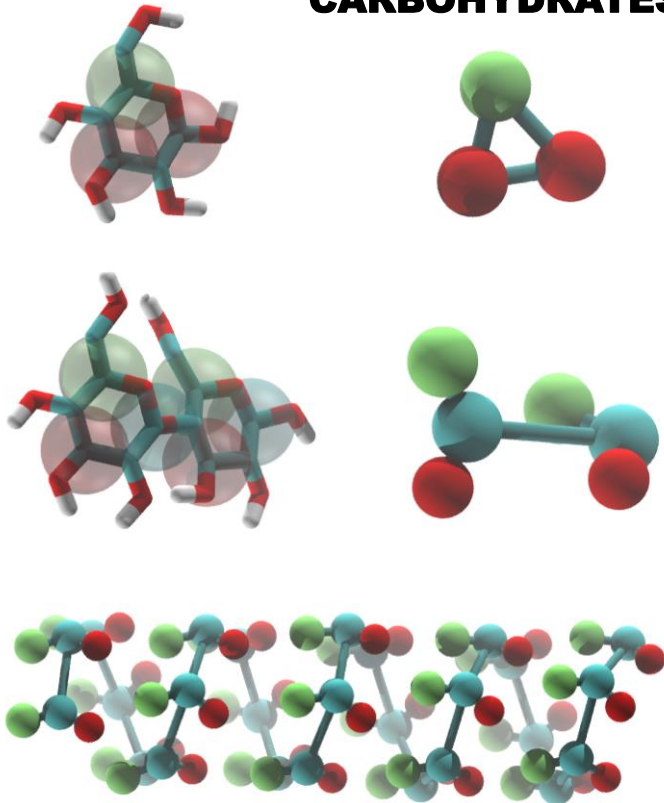
KOKEELLISEN TYÖN RAJOITUKSET



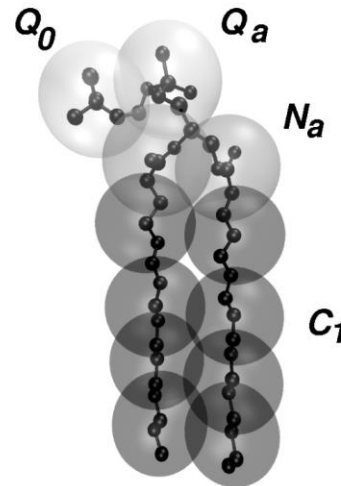
- Super-resoluutiomikroskopiolla (lähes) molekyylitason kuvantamista
- Resoluutio ~20-40 nm
- Nobel (mm. Stefan Hell) 2014

TARKEMPI RESOLUUTIO TIETOKONESIMULAATIOILLA

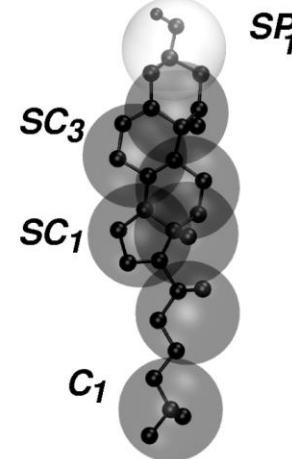
CARBOHYDRATES



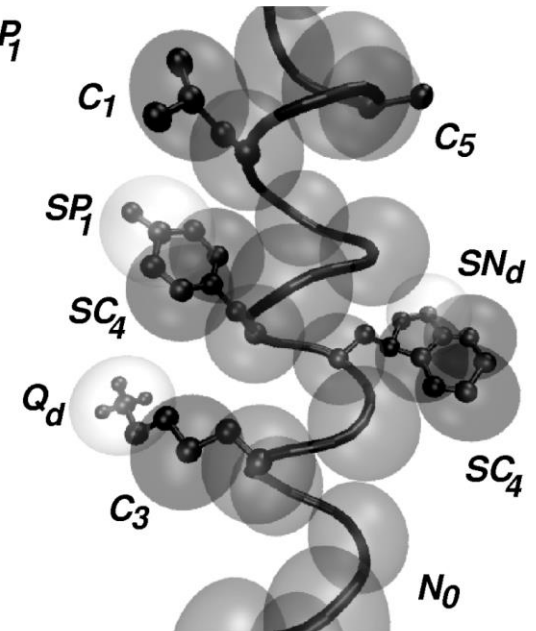
DPPC



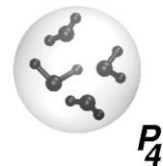
CHOLESTEROL



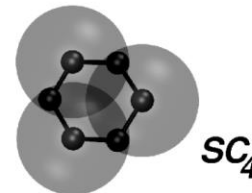
PEPTIDE (ALYWK)



WATER



BENZENE



State of the art:
~1,000,000 atomia
>1000 mikrosekuntia

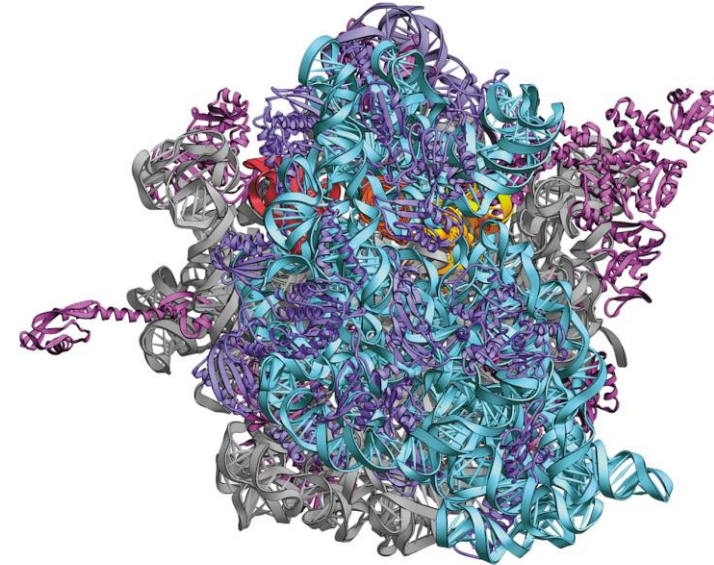
- Atomistiset OPLS, Charmm jne. voimakentät
- MARTINI-malli (Marrink, Groeningen)

RASKAS TYÖ TIETOKONEILLE...

$$m_i \ddot{\mathbf{r}}_i = \mathbf{f}_i \quad \mathbf{f}_i = -\frac{\partial}{\partial \mathbf{r}_i} \mathcal{U}$$

$$\mathcal{U}_{\text{non-bonded}} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] + \frac{Q_1 Q_2}{4\pi\epsilon_0 r}$$

$$\begin{aligned} \mathcal{U}_{\text{intramolecular}} = & \frac{1}{2} \sum_{\text{bonds}} k_{ij}^r (r_{ij} - r_{\text{eq}})^2 \\ & + \frac{1}{2} \sum_{\substack{\text{bend} \\ \text{angles}}} k_{ijk}^\theta (\theta_{ijk} - \theta_{\text{eq}})^2 \\ & + \frac{1}{2} \sum_{\substack{\text{torsion} \\ \text{angles}}} \sum_m k_{ijkl}^{\phi, m} (1 + \cos(m\phi_{ijkl} - \gamma_m)) \end{aligned}$$



ILMAN RESURSSSEJA EI OLE TIEDETTÄ



CSC – IT Centre for Science

- Cray XC30 + muut koneet
- Noin 40,000 corea

Muiden supertietokonekeskusten tarjoamat resurssit:

- Tier-0 resurssit (PRACE): mm. 60,000,000 core-tuntia (helmikuu 2013)
- Tier-0 projektit vastaavassa hengessä (2014-2016)
- Tier-1 resurssit (DECI/PRACE)
- Jugine (Julich)
- HorseShoe (Odense, Denmark)
- SharcNet (Canada)
- Jne.

Ryhmämme käytti ~15,000 core-vuotta laskentaresursseja vv. 2013-2014.