

First floor topics

- Does it matter where you go ?
 - one can change groups (in principle)
- what it means
 - seminar (small talk)
 - software project
 - masterarbeit
 - optional subjects (wahlpflicht)
- close contact with group members
- to do
 - talk to PhD students + students from last year

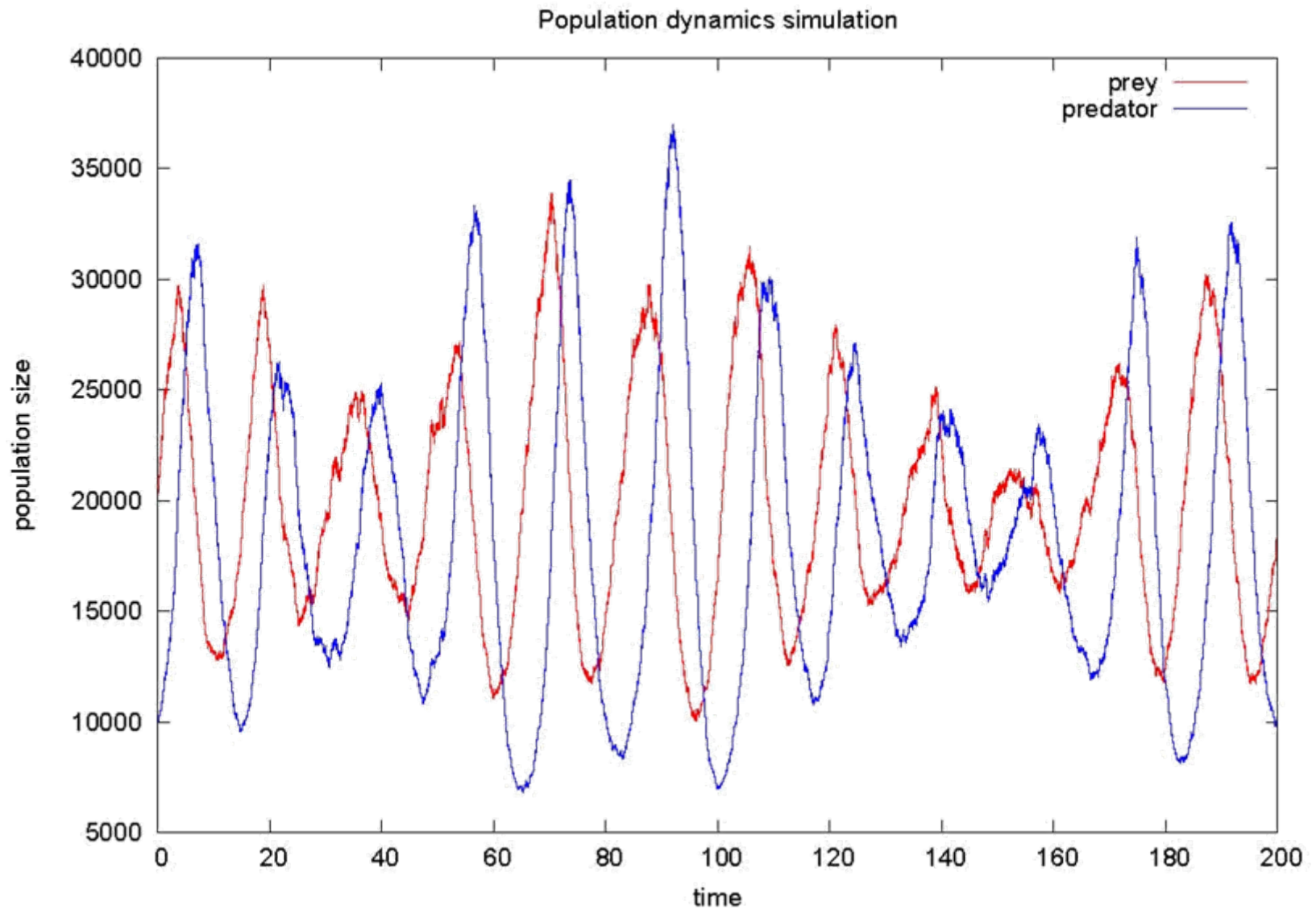
Names

- students who are still around
 - Björn Hansen, Jacques Kühl (projects and seminars now)
 - Birute Karsten (now with Rarey group)
 - Marvin Mundry (worked as HiWi)
- Doktoranden
 - Paul Reuter
 - Nasir Mahmood
 - Stefan Bienert
 - Gundolf Schenk
 - Thomas Margraf

- Seminars
 - anything
- Software projects
 - small groups, technical projects
- Mastersarbeit
 - 1 semester serious project
 - in one of our research areas / external projects
- Broad areas
 - evolution
 - RNA
 - protein simulation / comparison / prediction

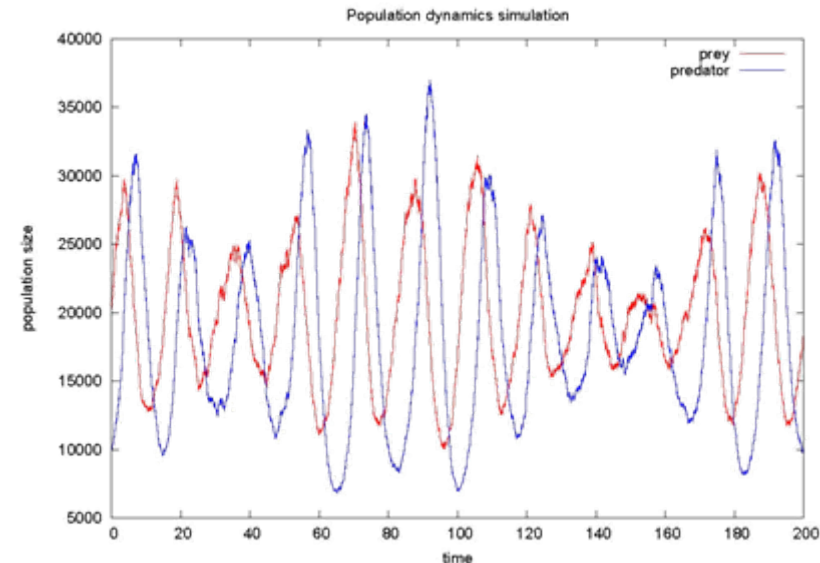
Evolution simulations

Paul Reuter



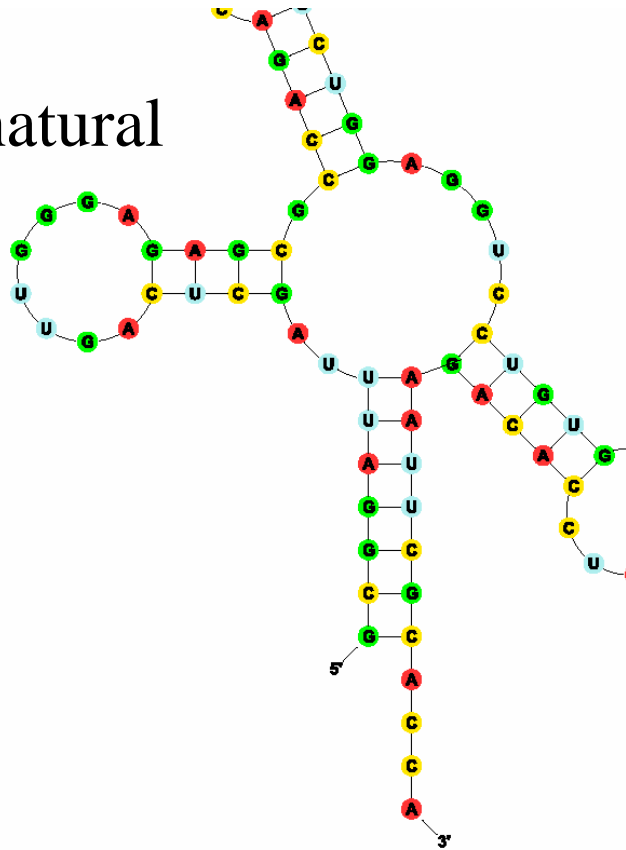
Evolution simulations

- Evolution applied to organisms ? No
- what makes a whole system evolve ?
- predator / prey, Hasen / Fuchs
 - do they evolve in isolation ?
- what is evolving ?
 - interaction parameters
- Paul's area
 - multi-level simulations
 - differential equations + high level search

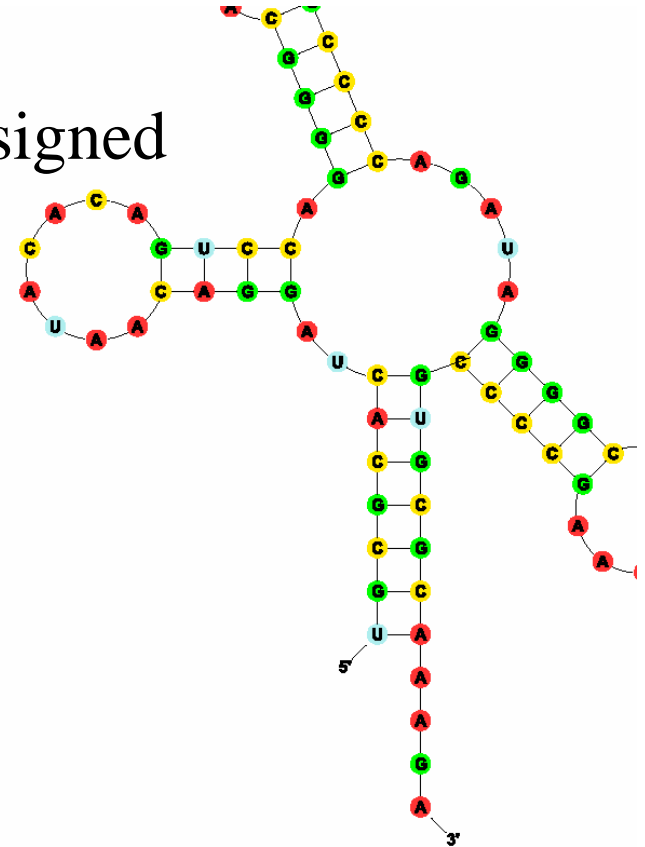


- Structure prediction
- Sequence design
- Work with biochemistry
 - finding riboswitches, sequence-based properties
- Side issues
 - drawing, pseudoknot removal
- Examples
 - structure prediction
 - sequence design

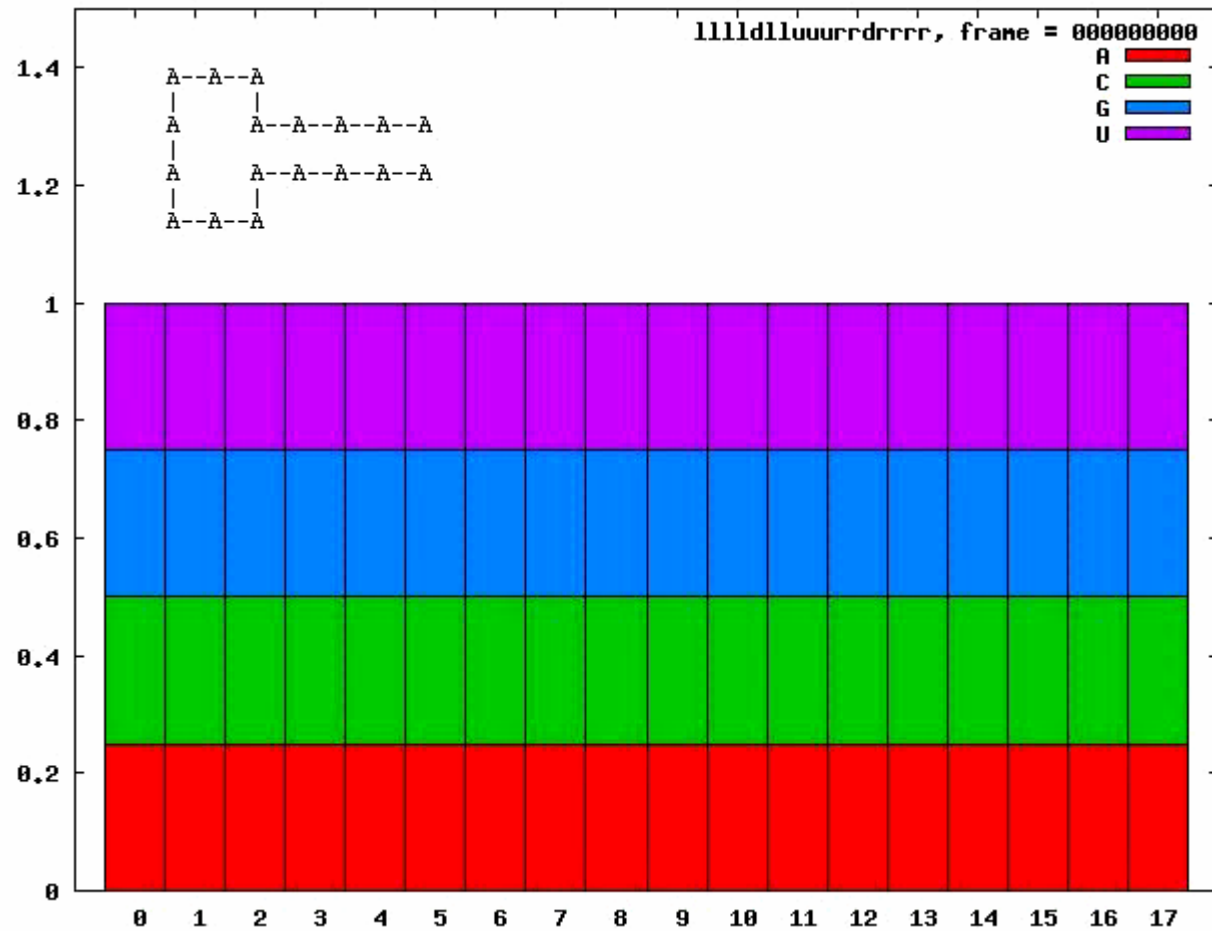
natural



designed



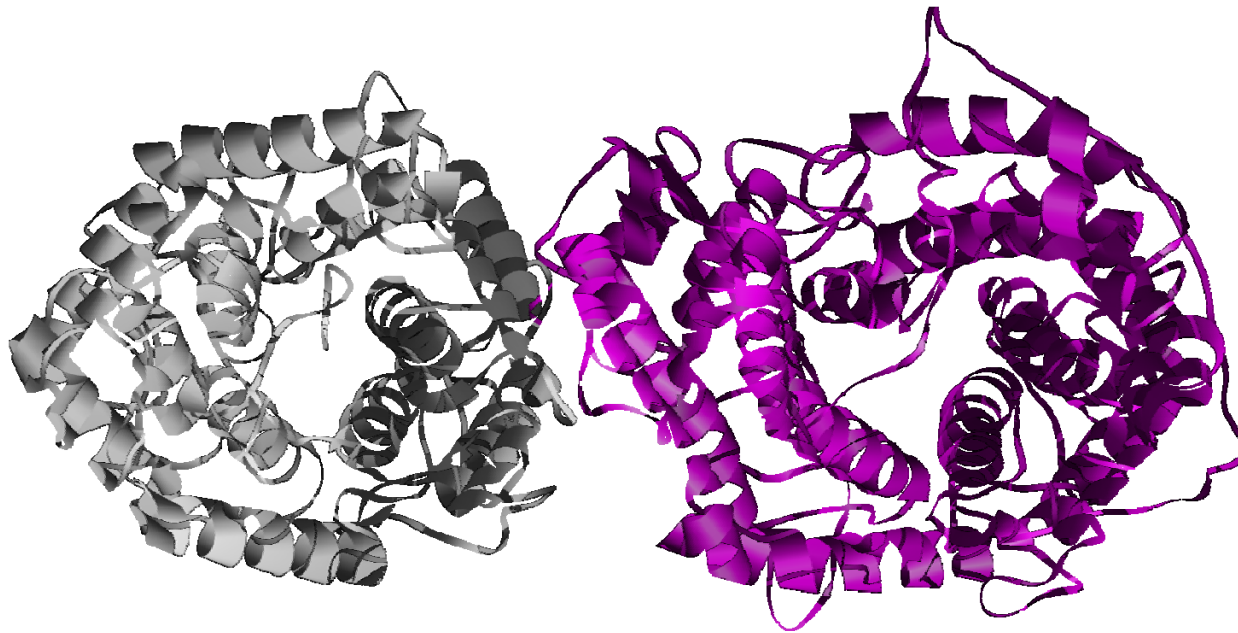
RNA

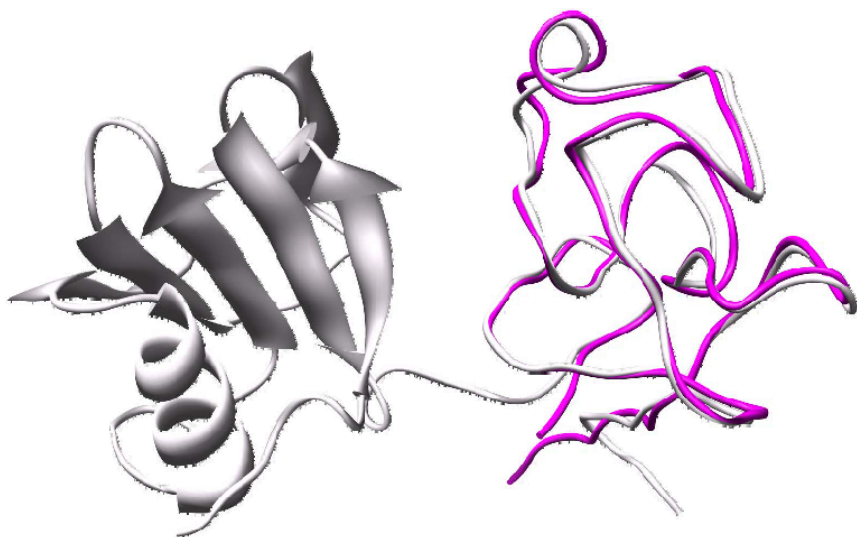
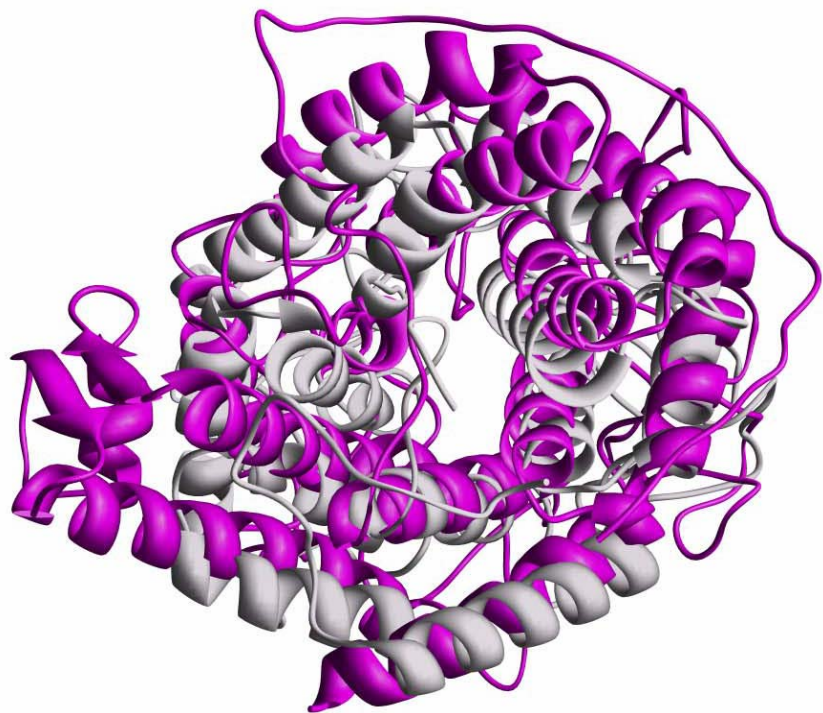


movie from Marco Matthies

Proteins

Gundolf Schenk
Nasir Mahmood
Thomas Margraf





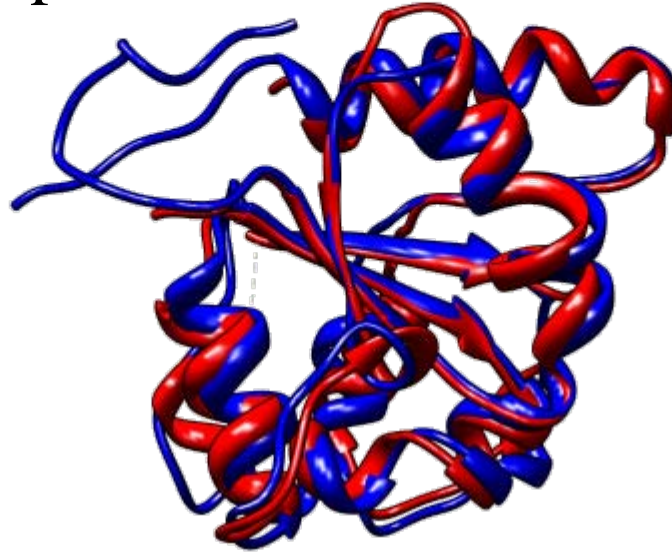
- very fast
- handles missing pieces..
- what is more interesting ?

Proteins

- TLR / toll-like receptors

48 % sequence id
1o77

another TLR



Proteins

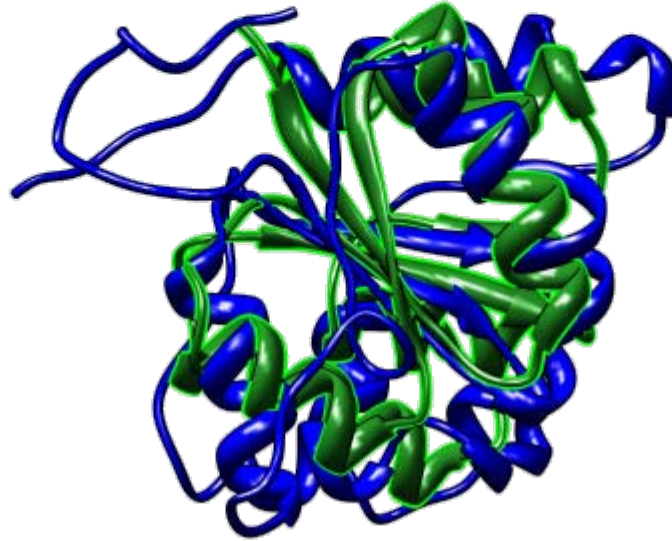
- TLR / toll-like receptors

6 % sequence id

2qxy

response regulator

T. Maritima

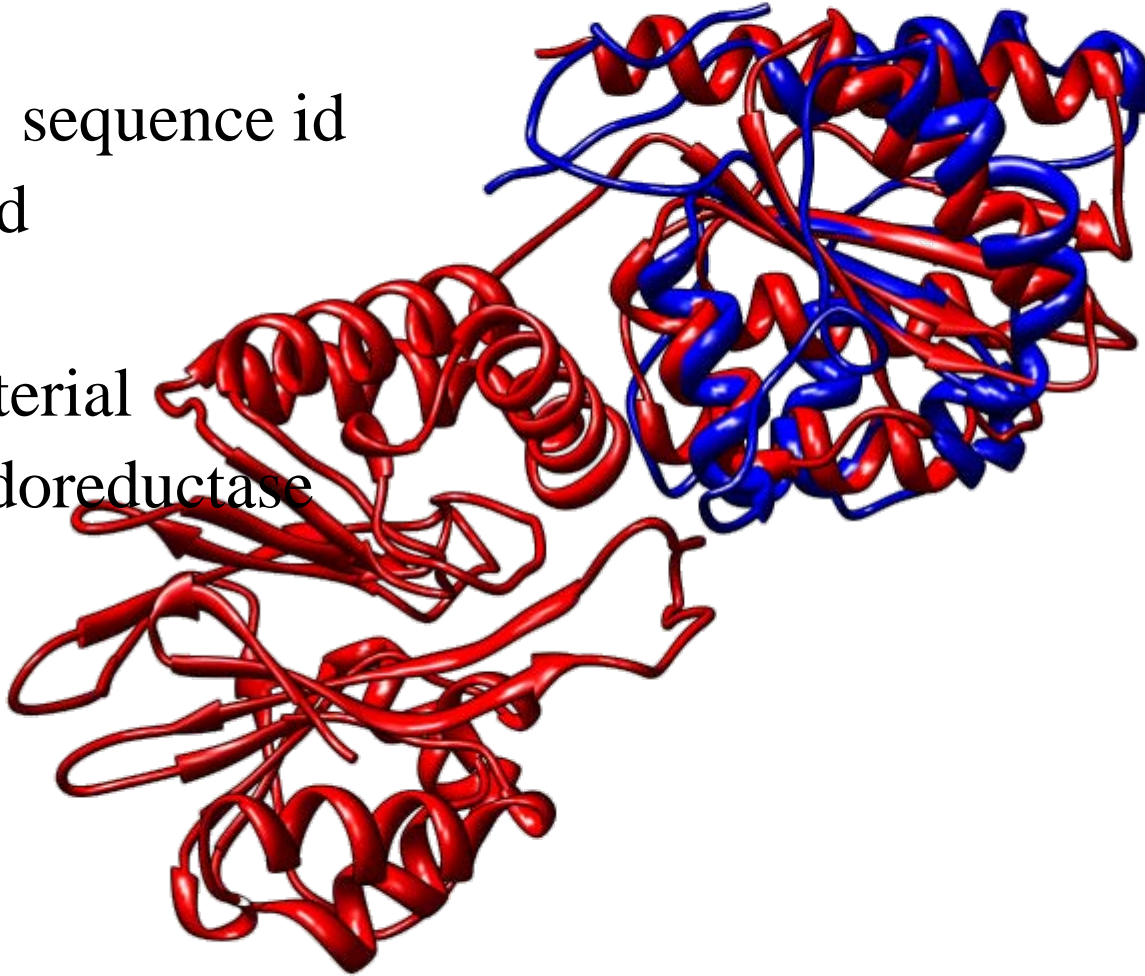


Proteins

- TLR / toll-like receptors

9 % sequence id
1e5d

bacterial
oxidoreductase



Proteins

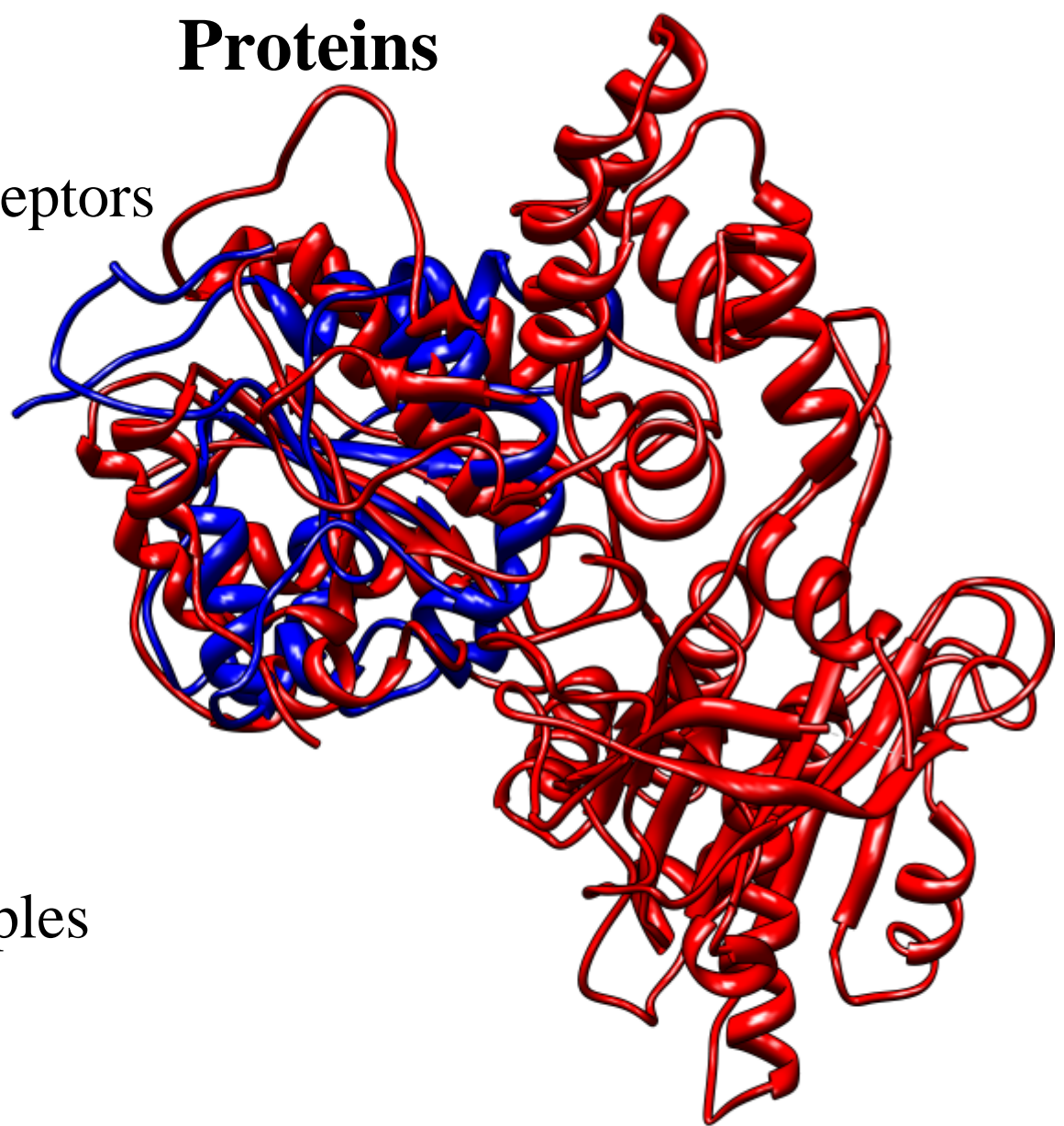
- TLR / toll-like receptors

7 % sequence id

1ja0

rat

oxidoreductase



- 100's more examples
- how are they calculated ?

Proteins

Jörn Lenz

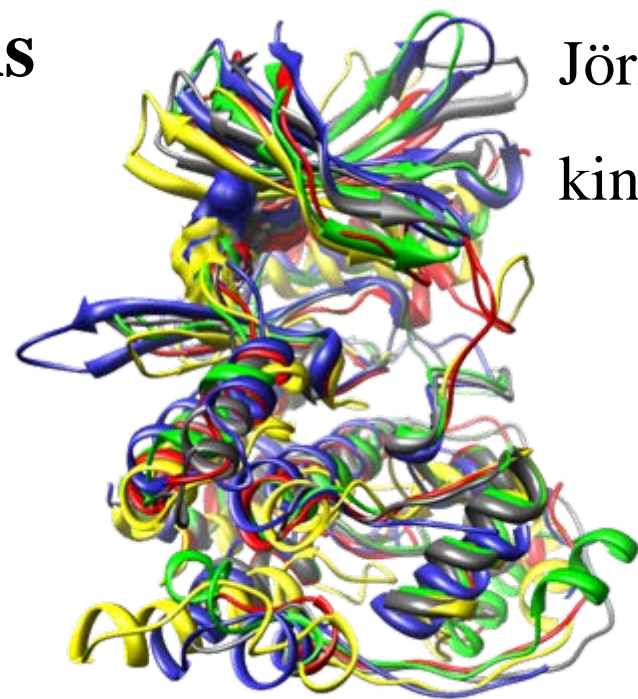
kinases

Research themes

- structural phylogenies
- structure prediction
- sequence design

Typical projects

- phylogeny / distance embedding
- force fields for structure prediction



```
1omwA ..TM.....N..D.F.S.V.H.....H.I.G.R.C.G.F.G.E.V..Y.G..C.R. 181
2srcA ..PR.....E..S.L.R.L.E.....V.K.L.G.C.C.F.G.E.V..W.M..G.T. 202
1lp4A W.G.E.Q....D...D.V.E.V.....K.V.C.R.C.K.Y.S.E.V..F.E..G.I. 51
1jklA ..V.D.....D...Y.Y.D.T.G.....E.E.L.G.S.C.Q.F.A.V.V..K.K..C.R. 30
1lufA .....V.D.I.C.E.G.A.F.G.R..V.F.Q.A.R. 33
1phkA .....I.....L.G.R.C.V.S.S.V.V.R.R..C.H.K.P. 26
1f3mC ..K.K.....K..Y.T.R.F.E.....K.I.G.Q.C.A.S.G.T.V.Y..T.A.M.D.V. 42
1cdkA ..K.E.....D...F.L.K.K.....W.E.N.P.A.Q.N.T.A.H..D.Q..F.E. 37
1kwpA ..S.G.....L...Q.I.K.K.....N.A.I.D.D.Y.K.V.T.S..Q.V..L.G. 26
1bowA ..K.D.....A...R.V.I.L.V.....K.L.G.C.H.F.S.T.V..W.L..A.K. 33
1b6cB ..A.A.....R...T.I.V.L.Q.....E.S.I.C.K.R.E.F.G.E.V..W.R..G.K. 49
1gngA ..Q.E.....V...S.Y.T.D.T.....K.V.I.C.N.C.S.F.G.V.V..Y.Q..A.K. 39
1a06A ..F.S.....E...V.I.L.A.E.....D.K.R.T.Q.K.L.V.A.K..C.I..A.K. 44
1csnA .....N.V.V.G.V..H.V.K.W.G.....R..R.I.C.E.G.S.F.G.V..I.F..E.G. 24
1hiwA ..P.Q.P..R.K.K..R.P.E.D.F.....K..F.C.K.I.L.G.E.G.S..F.S..T.V. 26
1hckA .....M.E.N..F.Q.K.W.E.....K..I.C.E.C.T.Y.G.V.V..Y.K..A.R. 22
1ir3A ..V.S...R.E.K..I.T.L.L.R.....E.L.G.C.C.S.F.G.M.V.V..E.G..N.A. 35
1tkiA ..I.Y...E.K.Y..M.I.A.E.D.....L.G.R.C.E.F.G.I.V.H.R..C.V..E.T. 27
1ia8A ..P.F..V.E.D.W.D..L.V.Q.T.L.....G.E.G.A.Y.E.V.Q.A..V.N..R.V. 29
1muoA .....R.P.L.G..G.K.F.C.N.V.V..A.R.E...K.Q. 27
1o6yA .....E.I.....L.G.F.G.C..S.E.V.H.L.A.R.D.L.R..L.H. 32
1jnkA ..V.L.....K.R.Y.Q.N..K.P...I.G.S.G.A.Q.I.V.C.A..Y.D.A.V..D.N. 44
1m14A ..K.E.....T.E.F.K.K..K.V.L.G.S.G.A.F.G.T.V.Y.K..L.V.I.P.E.G.E.K..V.K. 44
1gjoA ..D.P.....K.W.E.F.P.R.D.K..L.T.L.G.K.P.L.G.E.C.F.G.Q.V.V.M.A.E..A.V. 35
1o61A ..T.M.....N...D.E.D.Y.L..K.L.L.G.K.G.T.F.C.K.V.I.L.V.R.E.K.A..T.G. 30
```