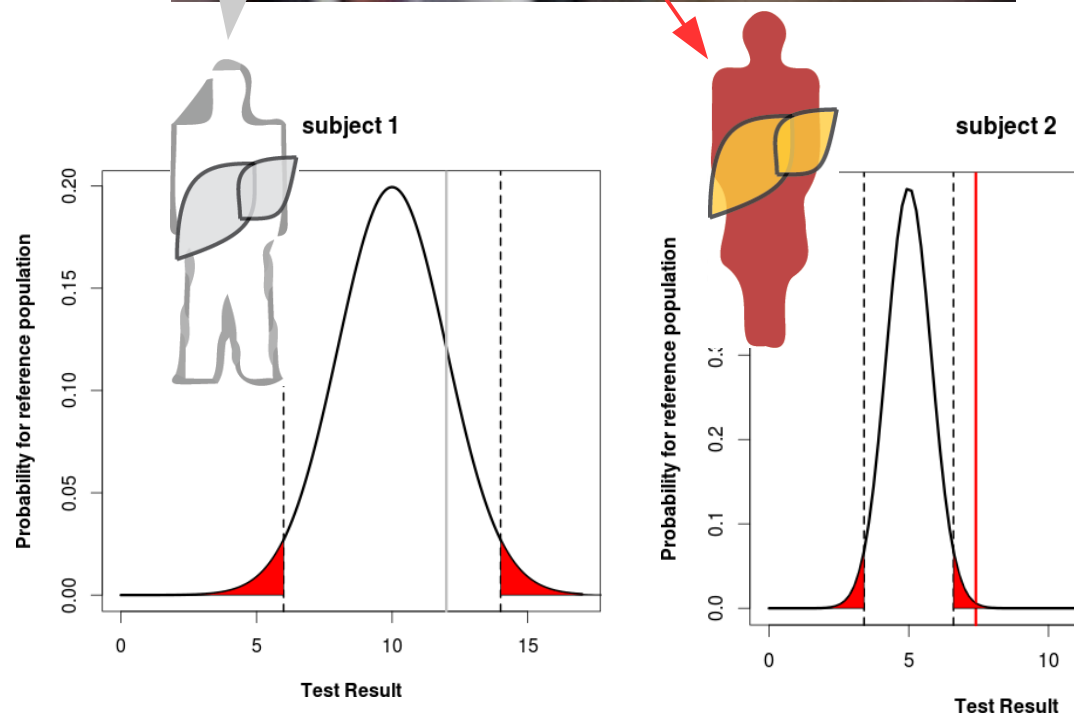


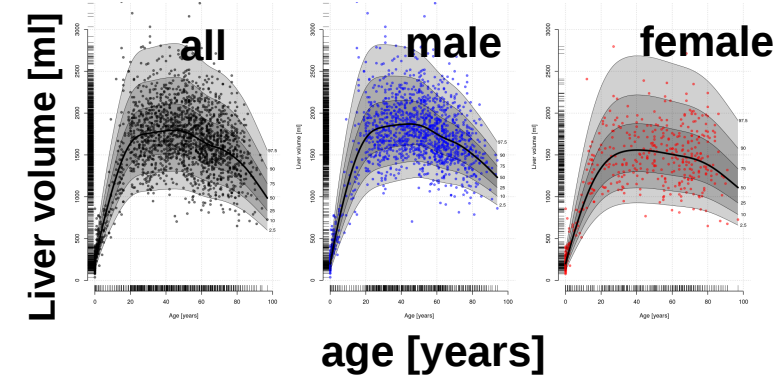
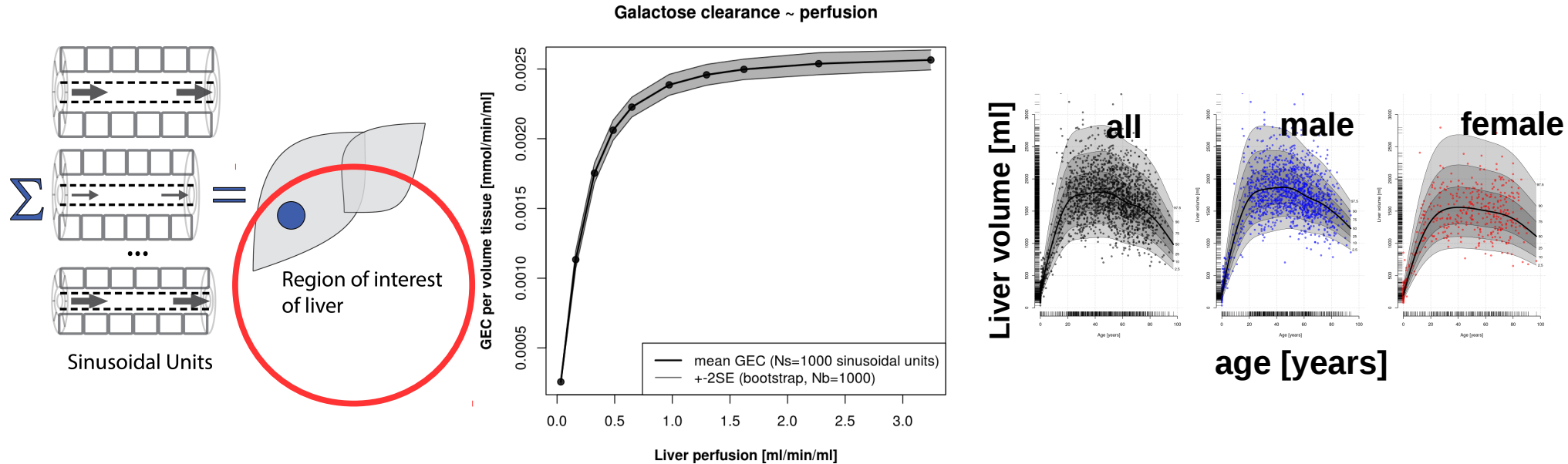
Individualized Liver Function

- Large population variability in liver volume & hepatic blood flow
 - Age, gender, bodyweight, height, ethnicity, ...
- Improved evaluation of liver function based on anthropomorphic data
 - Individualized liver function test
 - Reference range based on comparable individuals
 - Values outside range → further investigation & treatment
- Implementation
 - **Trainings data:** correlation between liver features and anthropomorphic data
 - **Prediction:** generalized additive models (nonlinear regression models)



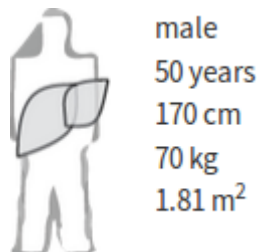
Individualized Liver Function

- Galactose elimination capacity (GEC) as proxy for liver function
- Tissue-Model predicts galactose clearance per tissue volume for given perfusion (**regional GEC**)
- Scale with predicted individual distributions of **liver volume** and perfusion (**total GEC**)
- Evaluation of individual & population variability in GEC

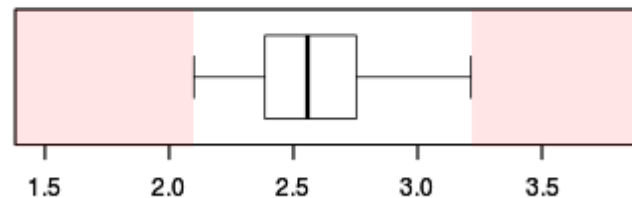


GEC Reference Range [2.5% - 97.5%]

[2.10 - 3.21] mmole/min
median 2.56



male
50 years
170 cm
70 kg
1.81 m²



GEC App



libRoadRunner: A High Performance SBML Simulation and Analysis Package

Endre T. Somogyi^{1,*}, Maciej Swat¹, James A. Glazier¹, Matthias König², Jean-Marie Bouteiller,³ and Herbert M. Sauro^{4,*} *

¹Biocomplexity Institute, Indiana University, Simon Hall MSB1, Bloomington, IN 47405

²Department of Computational Systems Biochemistry, University Medicine Charité Berlin, 10117 Berlin, Germany

³Biomedical Engineering Department, University of Southern California, Los Angeles, CA 90089

⁴Department of Bioengineering, University of Washington, Seattle, WA, 98195

(manuscript in submission)

libRoadRunner



Complex problems in computational biology **require highly efficient simulations, analyses or parameter optimizations** with thousands of cells and thousands of species and reactions in each cell.

- **Results**

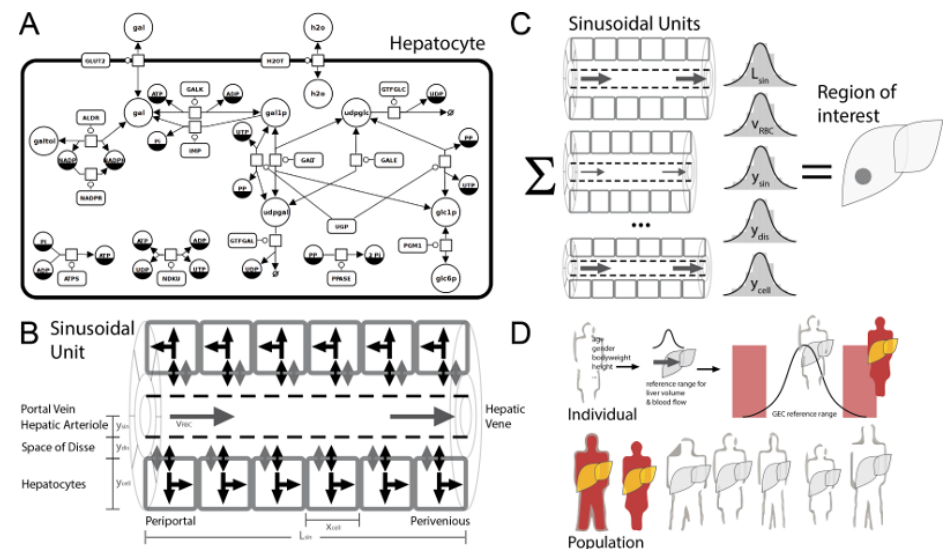
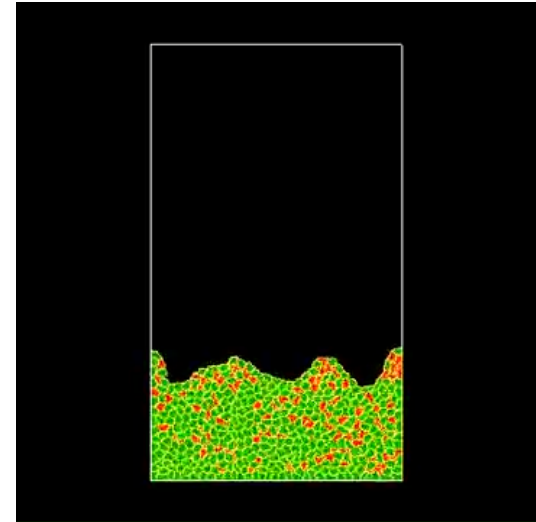
- Highly innovative cross-platform, open-source software library
 - easy integration with existing computational code
 - highly efficient
 - capable of handling very large and complex SBML models
- Uses novel just in time (JIT) compiler to compile SBML based models to optimized native machine code at runtime using LLVM
- Runs on x86 and ARM based processors
- Comprehensive native Python bindings
- Full suite of stoichiometric and metabolic control analysis routines

- **Availability & Implementation**

- Self-contained library with native C, C++ & Python bindings for Linux, Mac Os & Windows
- www.libroadrunner.org

LibRoadRunner Projects

- James A. Glazier, Biocomplexity Institute, Indiana University
 - Multi-cell simulation of tissue morphogenesis
 - CompuCell3D**
- Jean-Marie Bouteiller, Biomedical Engineering Department, University of Southern California
 - Large scale modeling of synaptic, neuronal and neuron network dynamics (**MEMORY** platform)
- Matthias König, Computational Systems Biochemistry
 - Multi-scale modeling of liver metabolism in **Virtual Liver Network**



Population Variability of Liver Function

König M. & Holzhütter HG.

