# Fundamentals of Simulation Methods

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SEIT 1386

Course at Heidelberg University
Winter Semester 2018/2019


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# About

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target audience:

- master students in physics & astronomy
- bachelor students welcome, but there is also a special bacelor module UKWR2 “Einführung in die Computerphysik”

- part of Computational Physics Specialization
- can be chosen as part of Master Specialization (MVMod)
- 8 credit points

# Requirements

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- you have basic knowledge of at least one programming language (preferred: Python or C)
- you have some basic programming skills
- you know at least one plotting software (or use the plotting capabilities of Python)
- you have an understanding of the basic physics and mathematics principles

- you want to learn how to simulate physical problems on a computer

# Objectives of the course

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- reach an active understanding of applicable numerical methods and algorithms
- endow you with the capacity to
  - identify and classify common numerical problems
  - solve basic physical problems with adequate numerical techniques
  - recognize range of validity of numerical solutions

# Topics

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- basic concepts of numerical simulations
- numerical techniques
- discretization of ordinary differential equations, integration schemes of different order
- N-body problems, molecular dynamics, collisionless systems
- discretization of partial differential equations
- finite element and finite volume methods
- adaptive mesh refinement and multi-grid methods
- matrix solvers and FFT methods
- Monte Carlo methods, Markov chains, applications in statistical physics

# Web pages

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- practice group system of department:
  https://uebungen.physik.uni-heidelberg.de/v/957
  please register for a group

- Moodle: details on login etc. will follow

- lecture notes, slides, and homework problem sets will be posted on course web pages

# Homework problems

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- Tutors: **Xudong Gao, Theodoros Soultanis, Peter Rodenkirch**

- tutorials will be given (one per week for each participant, three dates available: Thursday 11am – 1pm; 2pm – 4pm and Friday 11 am – 1pm) at CIP Phil 12

- registration for the three tutorial groups will be unlocked tomorrow (Friday, Oct. 19), 8am

- set will be made available on webpage every week starting next week
- you are welcome to bring your laptop, but desktop computers are available in the CIP pools

# Homework grading / exam

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- half of the homework exercises have to be solved
- submission of results is not mandatory

- attendance of all tutorials is mandatory (in case of illness etc. inform your tutor via email)

- a list will be provided, mark the problems that you have worked on
- you should be able to present your solution to any marked problem during the tutorial, each participant has to present ~2 problems

- written final exam, admission for all who have marked >50% of the homework problems

# Suggested reading

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## lecture notes

- lecture notes by Volker Springel (with updates by Cornelis Dullemond and Frauke Gräter) will largely be followed (but a few modifications are possible)
- available for download on course web page, together with slides shown in the lecture

## textbooks

- no additional literature strictly needed, but a great book to find more details is the classic

  Press, Teukolsky, Vetterling & Flannery: *"Numerical Recipes"* (different editions, versions for various programming languages, see http://numerical.recipes/, some older versions available for free online reading)

# Schedule (may change!)

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October

- 16. 10. (Röpke) Intro, numbers in numerics
- 18. 10. (Röpke) numbers in numerics, solving simple equations
- 23. 10. (Röpke) integration of ODEs
- 25. 10. (Röpke) integration of ODEs
- 30. 10. (Dullemond) collisionless particle systems

November

- 1. 11. Public holiday
- 6. 11. (Dullemond) Tree algorithms
- 8. 11. (Dullemond) Tree algorithms
- 13. 11. (Dullemond) Particle-Mesh method
- 15. 11. (Dullemond) Particle-Mesh method
- 20. 11. (Dullemond) Force calculation with Fourier methods
- 23. 11.  (Dullemond) Force calculation with Fourier methods
- 27. 11. (Röpke) Iterative solvers, multigrid
- 29. 11. (Röpke) Iterative solvers, multigrid

# Schedule (may change!)

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December

- 4. 12. (Röpke) MD simulations
- 6. 12. (Röpke) MD simulations
- 11. 12. (Röpke) Monte Carlo methods
- 13. 12. (Röpke) Monte Carlo methods
- 18. 12. (Dullemond) Basic gas dynamics
- 20. 12. (Dullemond) Basic gas dynamics

January

- 8. 1. (Dullemond) Eulerian hydro
- 10. 1. (Dullemond) Eulerian hydro
- 15. 1. (Dullemond) SPH
- 17. 1. (Dullemond) SPH
- 22. 1. (Dullemond) Finite element methods
- 24. 1. (Dullemond) Finite element methods
- 29. 1. (Röpke) Parallelization
- 31. 1. (Röpke) Parallelization

Exam: 1$^{st}$ week of February

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# 0. Introduction

# Numerical simulations

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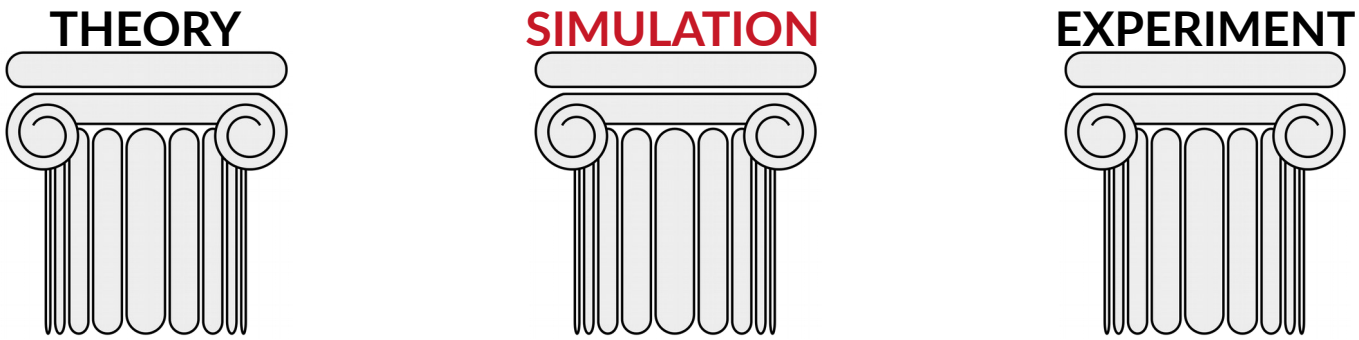
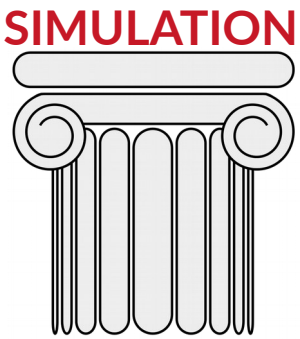
- natural sciences: Physics, Chemistry (Biology?) → three basic pillars have established (or are about to establish):

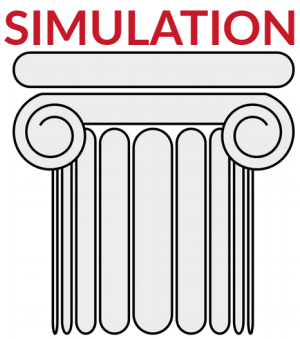


# Numerical simulations




- simulation involves aspects of both theory and experiment:
  - theory
    - theory models form the basis
    - often have to be simplified, approximated to be accessible to numerical approaches
    - discretization,choice of algorithms, numerical implementation (involves further approximation)
  - exp.
    - simulation on computer, perhaps multiple runs with changing parameters...
    - simulation results → data analysis
- advantage of simulations:
  - can be more realistic than analytic theory
  - allows better insight than experiments (data available almost anywhere at any point in time

# Numerical simulations




- simulation involves aspects of both theory and experiment:
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  - simulation results → data analysis

# Typical approach

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- theoretical model based on fundamental physical laws
- usually formulated in terms of PDEs or ODEs → mathematics

- discretize differential equations → numerical mathematics
- solve discretized equations with suitable algorithm → numerical modeling
- test numerical code for standard problems with known solution → validation

- set up target problem (with suitable boundary/initial conditions)
- run simulation(s)

- analyze output data → plotting, visualization…
- interpret results (paying attention to numerical errors)

# Cosmological simulation



- "Aquarius" (Springel+, 2008) → formation of milky-way sized dark matter halo of a galaxy in full cosmol. context → N-body simulation
- based on Poisson-Vlasov system (→ collisionless Boltzmann equation with gravity as external force):

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \vec{x}} \cdot \vec{v} + \frac{\partial f}{\partial \vec{v}} \cdot \left( -\frac{\partial \Phi}{\partial \vec{x}} \right) = 0$$

$$\nabla^2 \Phi(\vec{x}, t) = 4\pi G \int f(\vec{x}, \vec{v}, t)\, \mathrm{d}\vec{v}$$

# Cosmological simulation



- "Auriga" (Grand+ 2017) → add gas, magnetic fields

$$\nabla^2\Phi = 4\pi G\rho$$

$$\vec{g} = -\nabla\Phi$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = 0$$

$$\rho\left(\frac{\partial\vec{v}}{\partial t} + \vec{v}\cdot\nabla\vec{v}\right) + \nabla P - \rho\vec{g} - \frac{1}{\mu_0}(\nabla\times\vec{B})\times\vec{B} = 0$$

$$\frac{\partial P}{\partial t} + \vec{v}\cdot\nabla P + \gamma P\nabla\cdot\vec{v} = 0$$

$$\frac{\partial\vec{B}}{\partial t} - \nabla\times(\vec{v}\times\vec{B}) = 0$$

$$\nabla\cdot\vec{B} = 0$$

...and many kinds of source terms (modeling radiative cooling, star formation, supernovae, stellar winds, black holes and AGN, galactic winds...)

# Thermonuclear supernova explosion



- Delayed detonation in a carbon-oxygen white dwarf (Röpke+ 2008) → A model for Type Ia supernova explosions?
- (roughly) based on equations of reactive fluid dynamics with diffusion and heat conduction

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$$

$$\frac{\partial (\rho X_i)}{\partial t} + \nabla \cdot (\rho X_i \vec{v}) = -\nabla \cdot \left( \rho \vec{v}_i^{\,\mathrm{D}} X_i \right) + \rho \omega_{X_i}, \qquad i = 1, \ldots, N$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \rho \vec{v} \otimes \vec{v} + \nabla p = -\rho \nabla \Phi$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho E \vec{v}) + \nabla (p \vec{v})$$

$$= -\rho \vec{v} \cdot \nabla \Phi - \rho \sum_{i=1}^{N} X_i \vec{v}_i^{\,\mathrm{D}} \cdot \nabla \Phi - \nabla \cdot \left( \rho \sum_{i=1}^{N} h_i \vec{v}_i^{\,\mathrm{D}} X_i - \sigma \vec{\nabla} T \right) + \rho S$$

# Molecular dynamics simulation

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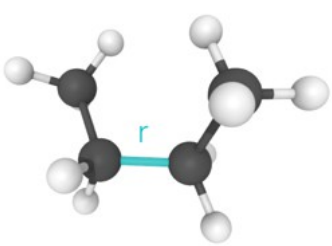
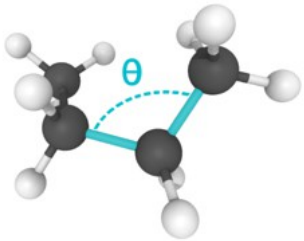
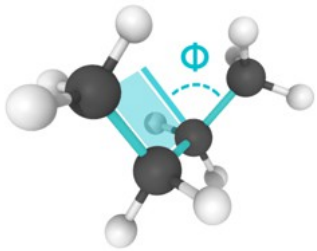
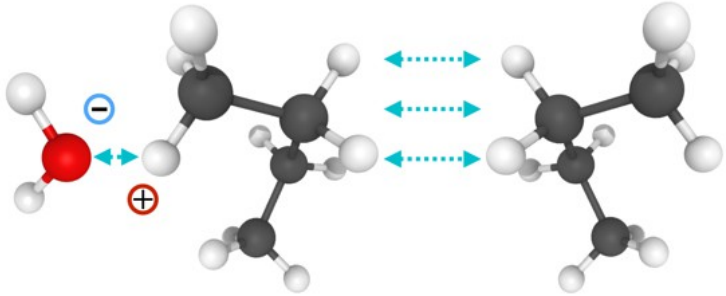
- simulation of multiple lipid bilayers that are successively broken by an external force (tip of atomic force microscope pressing on the membrane with constant force) (Franz+ 2018)
- based on Newton's second law

$$m_i \frac{\mathrm{d}^2}{\mathrm{d}t^2} \vec{r}_i = \vec{F}_i \; - \nabla_i U(\{\vec{r}_j\})$$

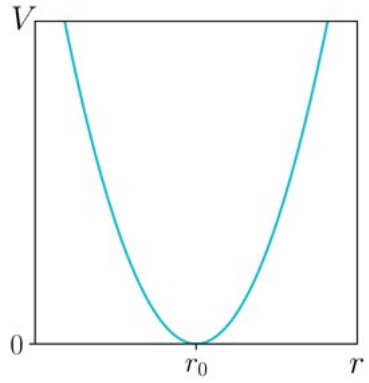


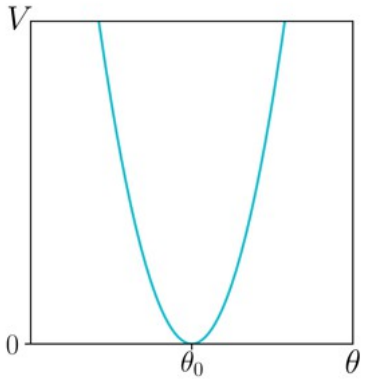



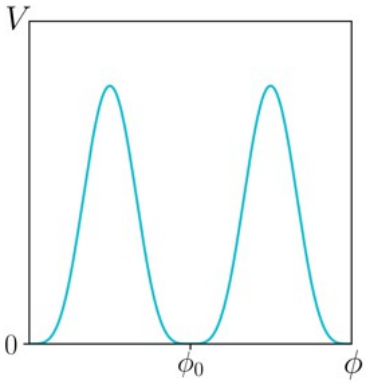



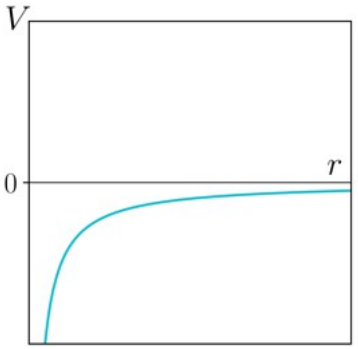



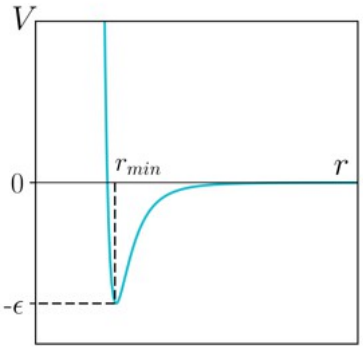
bond stretching | angle bending | dihedral torsion | electrostatics | van der Waals




F. Franz

# Student Cluster Competition 2019

| | |
|---|---|
| **The challenge:** | Build small HPC cluster within 3kW power consumption, optimize system and software, defeat the international competition :-) |
| **Next meetings:** | Monday, 22. 10. 2018, URZ, Raum 101, 16:30<br>Friday, 26. 10. 2018, URZ, Raum 101, 16:00 |
| **Supervision:** | URZ and EMCL employees |
| **Where?** | In Frankfurt at the International Supercomputing Conference 2019 |
| **When?** | 16.06.2019 to 20.06.2019 |
| **Why?** | Get to know cool people, get contacts, learn new skills, experience, play with brand-new HPC hardware and loads of fun :-) |
| **More information:** | http://hpcadvisorycouncil.com/events/student-cluster-competition/ |

**Come and join the team!**

URZ UNIVERSITÄTS-RECHENZENTRUM

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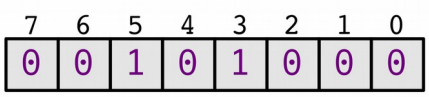
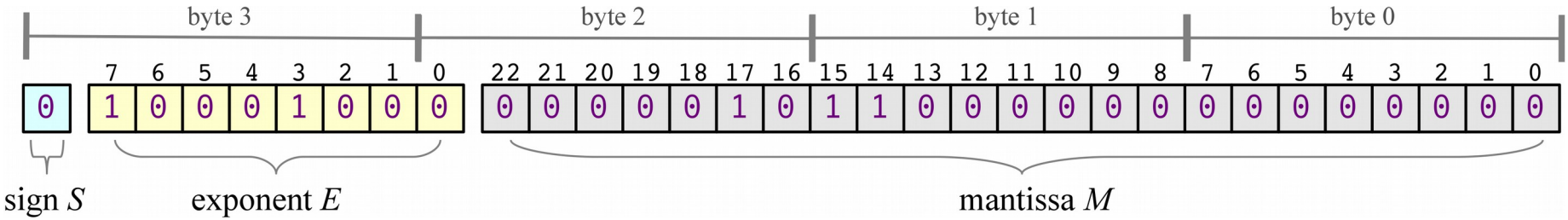
# Numbers in numerics



- byte




- IEEE-754 single precision storage scheme



# Single precision floating point numbers

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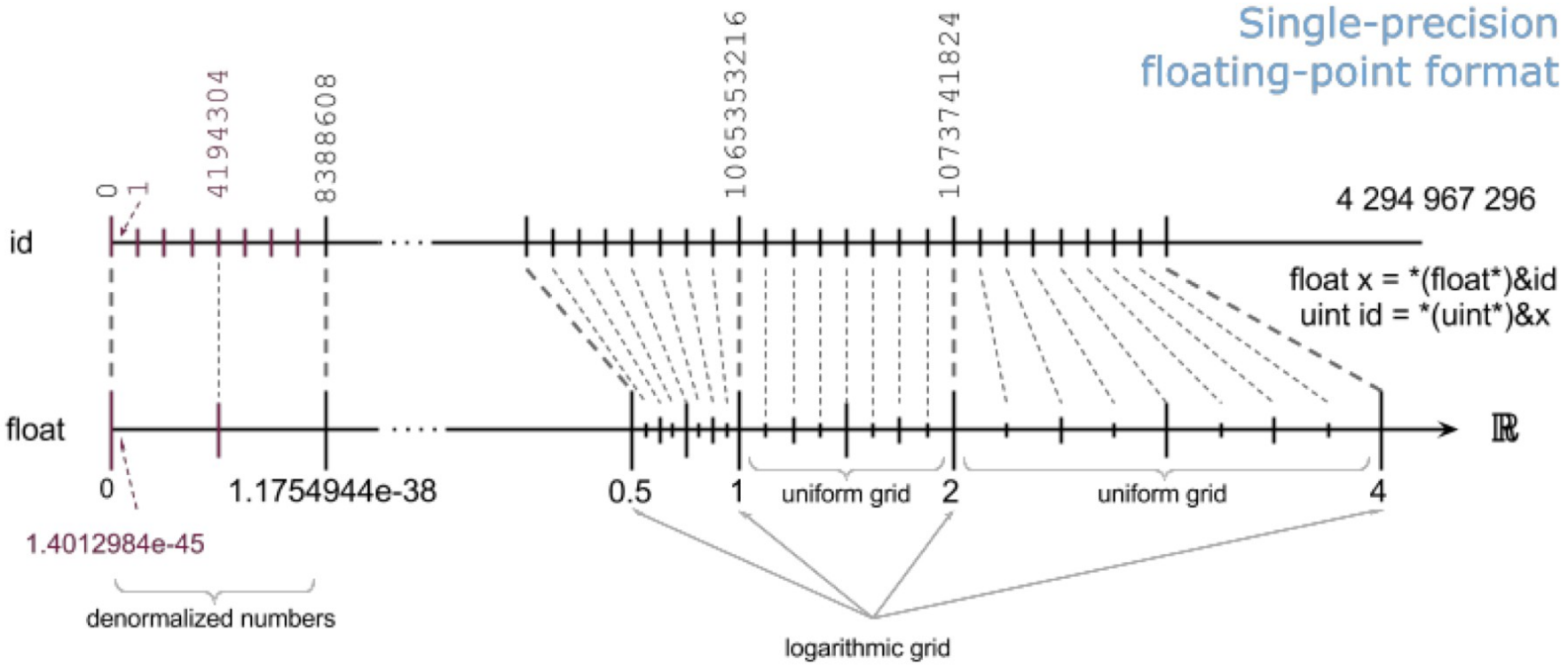
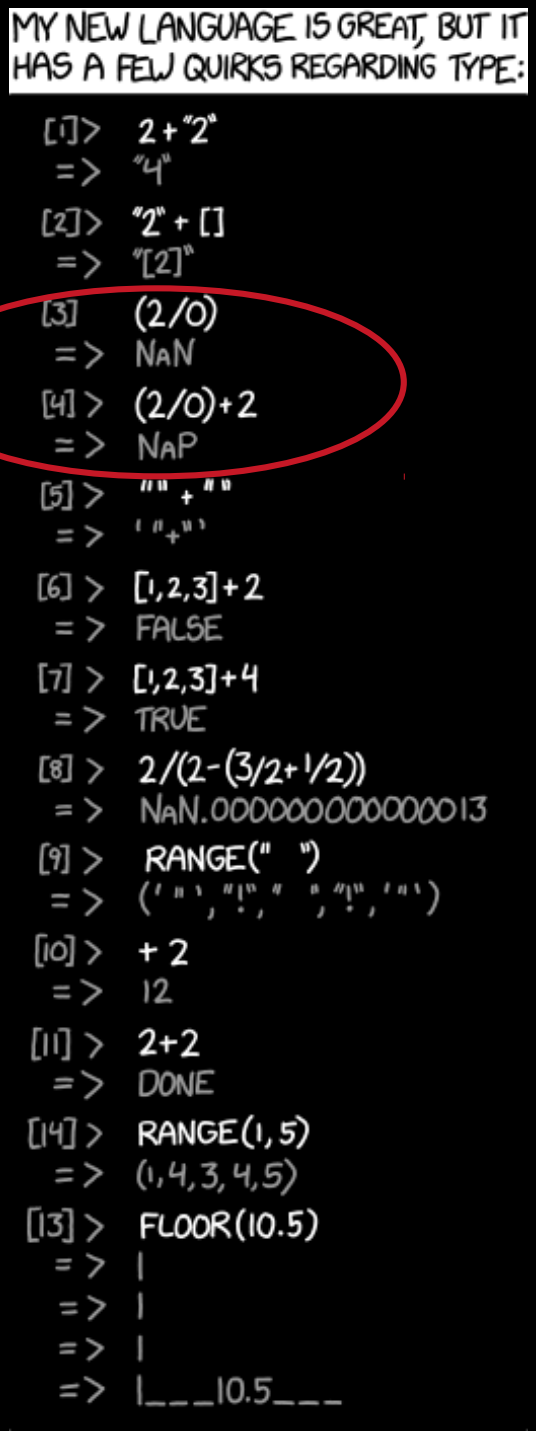
- set of representable IEEE-754 single-precision floating point numbers (figure by Denis Yurin)

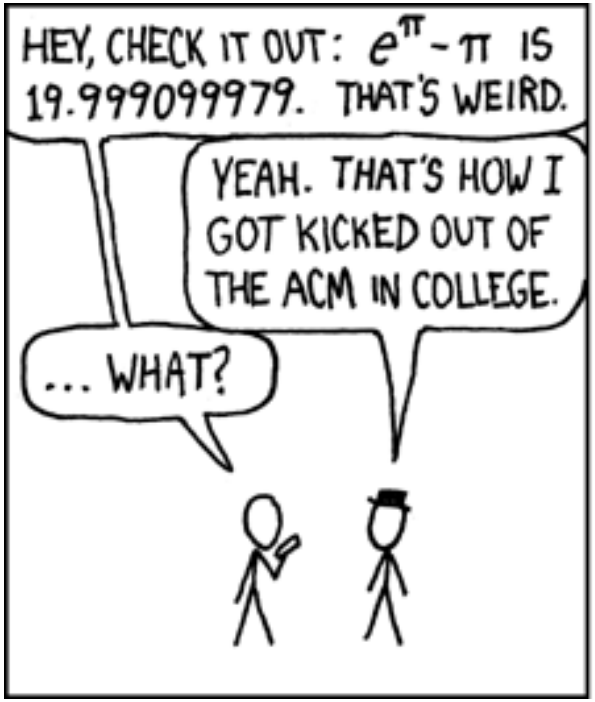


# xkcd on Floating point numbers...

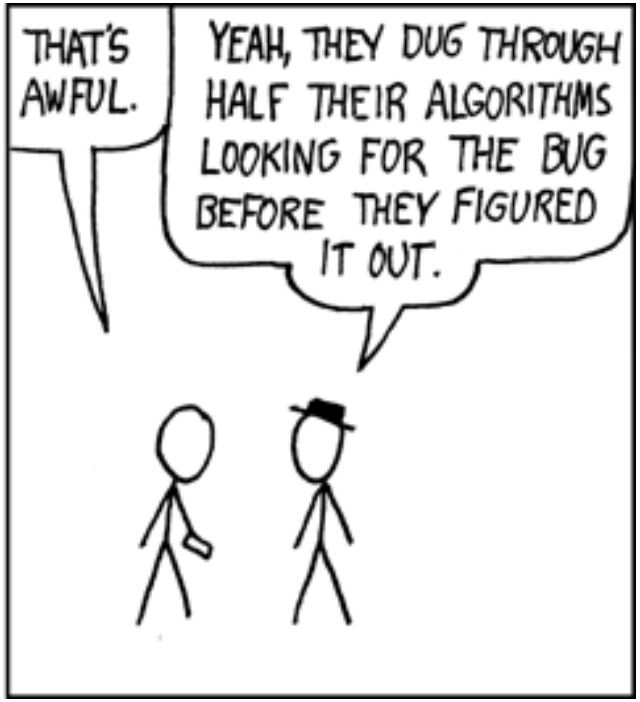


# xkcd on rounding errors...









# Euler method

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- Leonhard Euler (1707 – 1783)

INSTITVTIONVM
CALCVLI INTEGRALIS
VOLVMEN PRIMVM

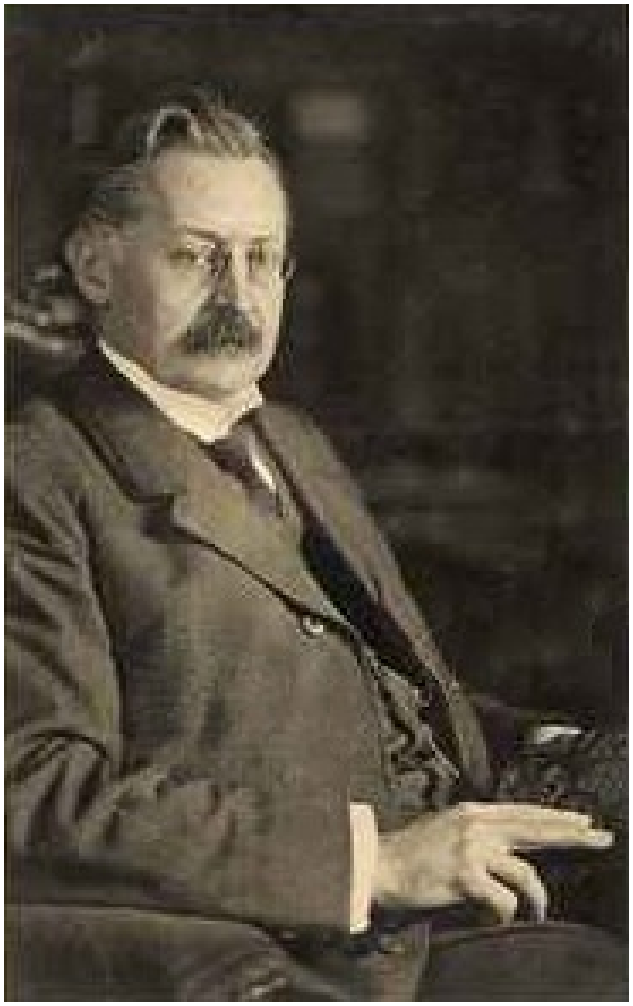
IN QVO METHODVS INTEGRANDI A PRIMIS PRINCIPIIS VSQVE AD INTEGRATIONEM AEQVATIONVM DIFFERENTIALIVM PRIMI GRADVS PERTRACTATVR.

AVCTORE
LEONHARDO EVLERO
ACAD. SCIENT. BORVSSIAE DIRECTORE VICENNALI ET SOCIO
ACAD. PETROP. PARISIN. ET LONDIN.

PETROPOLI
Impensis Academiae Imperialis Scientiarum
1768.

# Runge–Kutta methods





Carl David Tolmé Runge (1856 – 1927)

Martin Wilhelm Kutta (1867 – 1944)