On the impact of quantum computing technology on future developments in high-performance scientific computing

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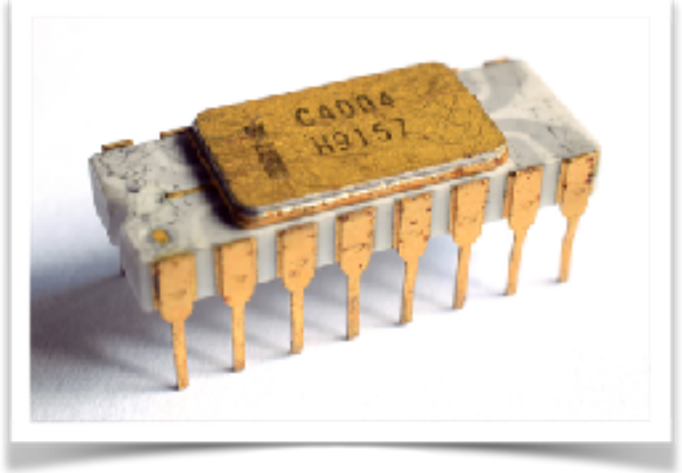
Outline

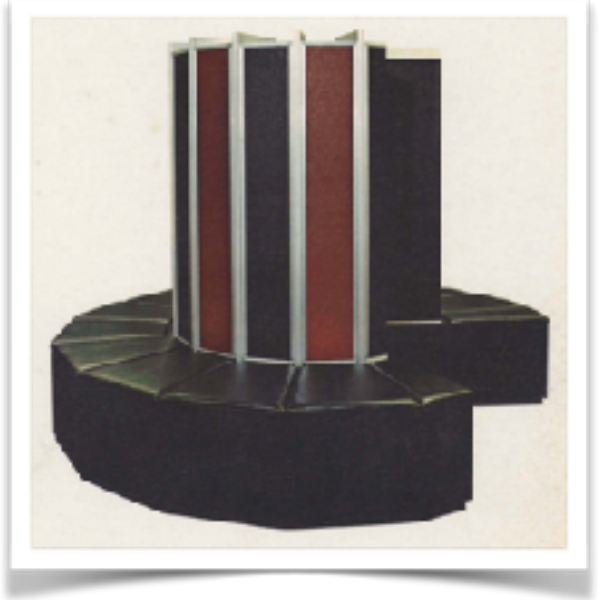
- High-performance scientific computing
  - Past, present and possible future trends
  - FEM making friends with exotic hardware

- Q-accelerated scientific computing
  - Potential use case examples
  - Challenges and open problems

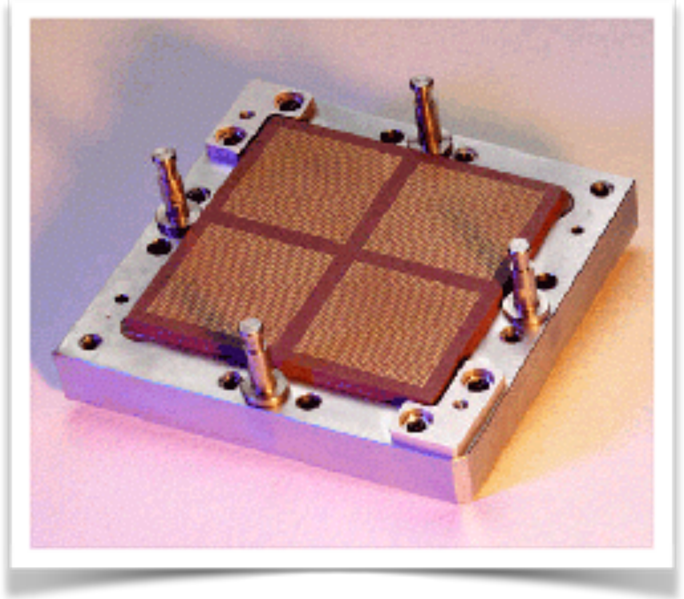
History of computing



1971: Intel 4004 first
commercial microprocessor



1976: Cray-1
first vector processor

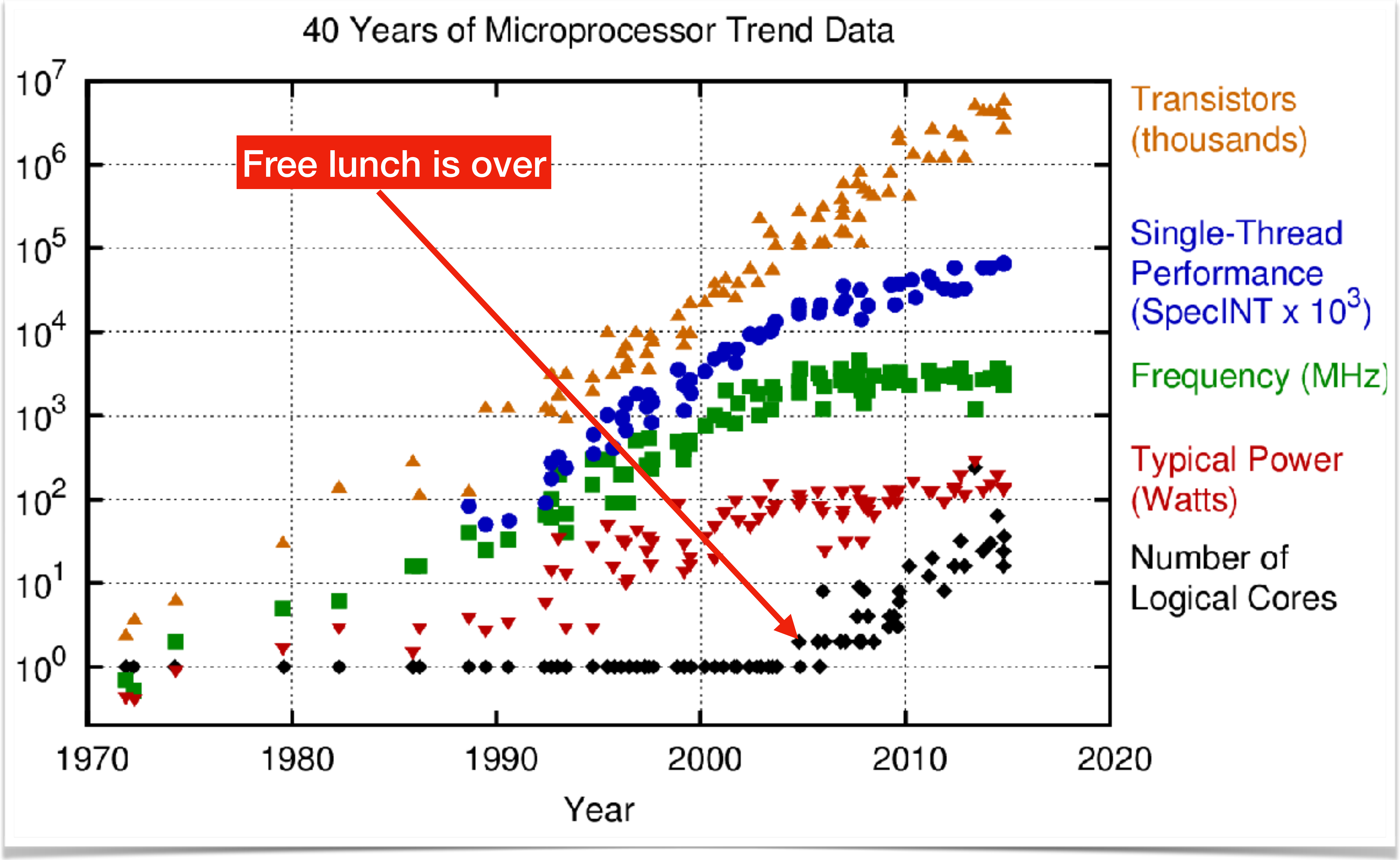


2001: IBM Power4
first multi-core CPU

2017: Intel Xeon Platinum
28 cores and AVX-512

- Redesign of algorithms is mandatory to exploit compute capabilities of modern hardware (multi-threading, vectorisation)
- “Algorithm follows hardware”

History of computing



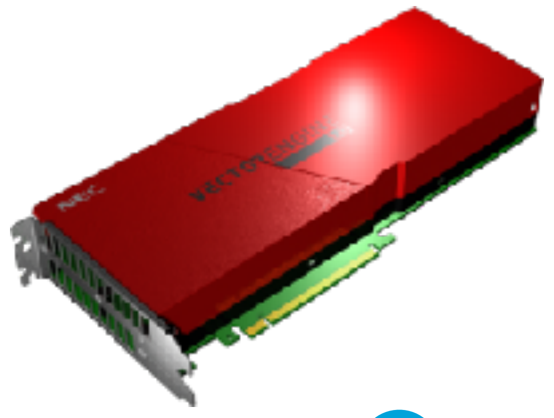
Credit: K. Rupp, 2015

History of accelerated-computing

1999: GeForce 256
“the world’s first GPU”

2006: GeForce G80
first CUDA-capable GPU

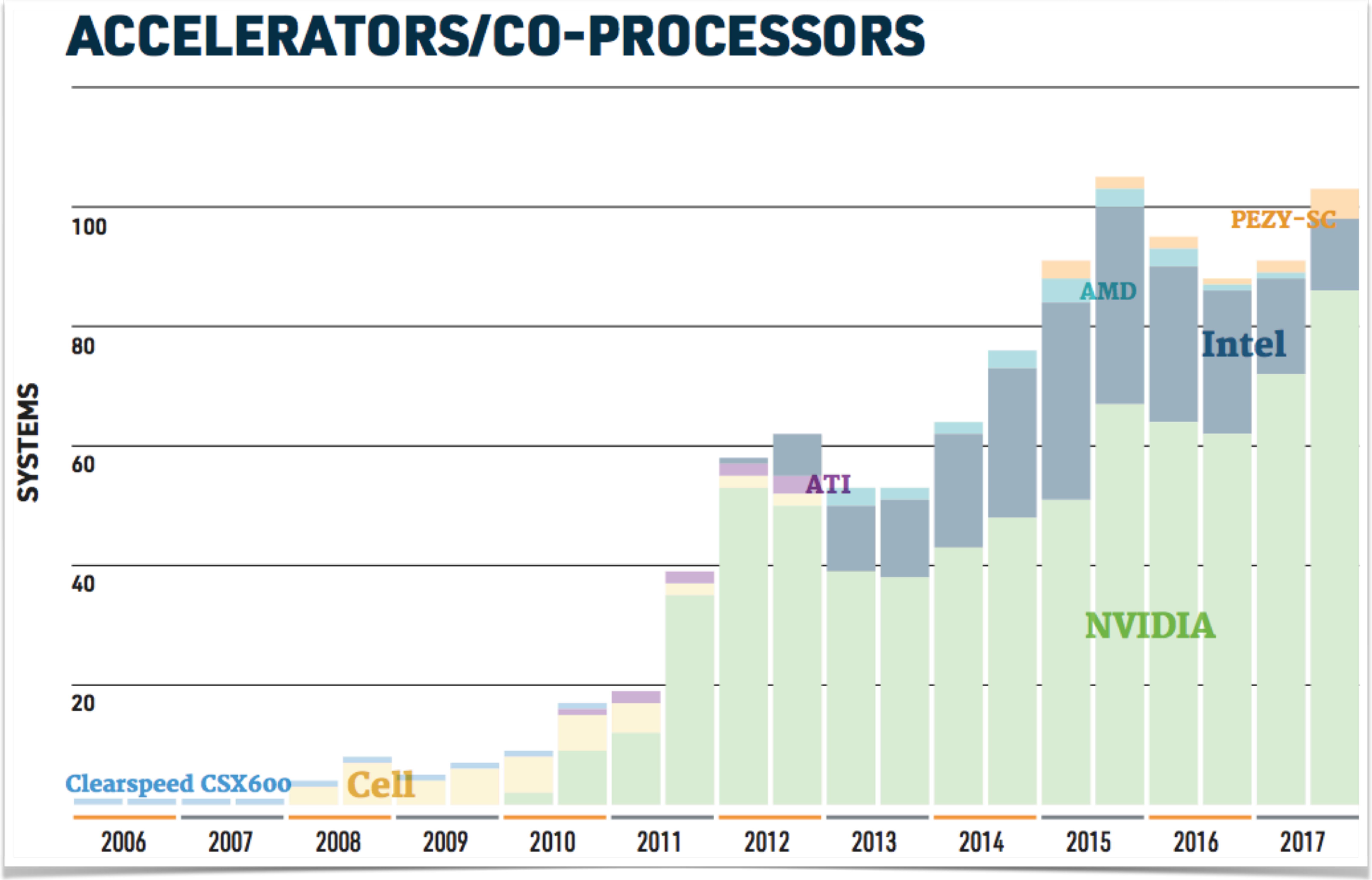
2013: Intel Xeon Phi



2017: NEC
SX-Aurora

2017: Tesla V100

History of accelerated-computing



Credit: TOP500, Nov 2017

History of accelerated-computing

1999: GeForce 256
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2006: GeForce G80
first CUDA-capable GPU

2012: Maxeler Technologies
FPGA-based DataFlow Engine
(Maximum Performance Comp.)

2013: Intel Xeon Phi

2016: Google TPUs (ML)

2017: NEC
SX-Aurora

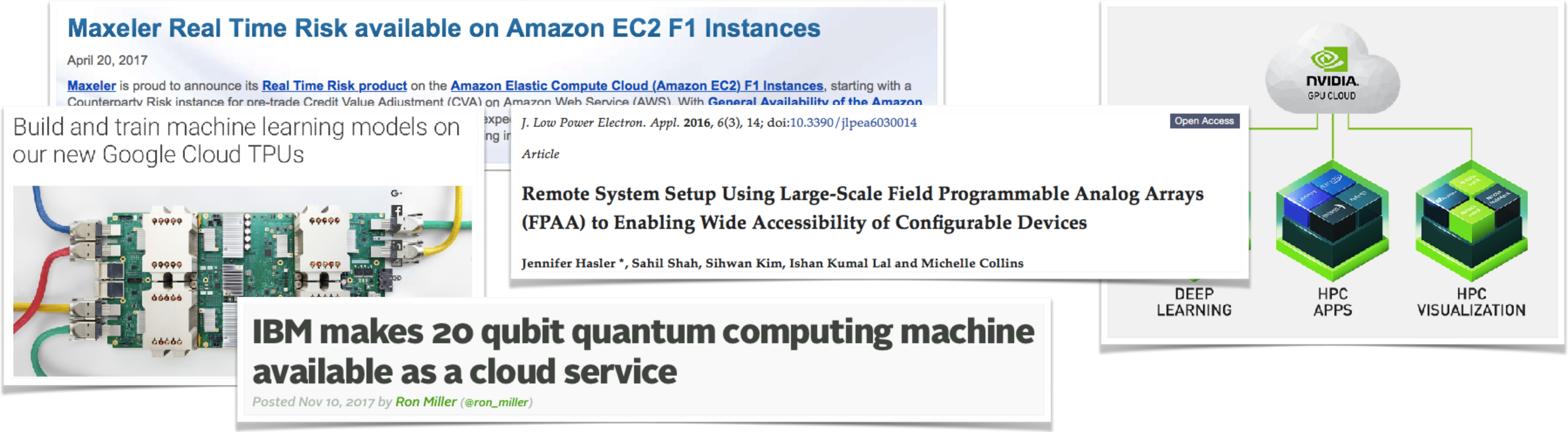
2017: Tesla V100
Tensor Cores (ML)

20??: HIVE

- Accelerated-computing is mainstream but still requires redesign of algorithms
- Application-specific hardware designs are becoming more popular paving the way for special-purpose functional acceleration
- “Hardware follows application”

Future trends in scientific computing

- Heterogeneous (most probably cloud-based) HPC clusters
  - multi-core/socket CPU-based host nodes
  - general-purpose many-core accelerators (GPUs, MICs, VPs)
  - special-purpose functional accelerators (TPUs, FP{G,A}As, QC?)



Future trends in scientific computing

- Expected paradigm shifts (“*since the free lunch is over*”)
  - closer co-design of compute hardware and applications
  - more fine-grained application-specific solution algorithms
  - new concepts like in-memory-computing, computing in space
  - rediscovery of ‘old’ approaches
    - *mixed-precision:* Wilkinson ’63, Strzodka et al. ’08, NVIDIA ’16
    - 

The Finite Element Method

From textbook version to HPC implementation

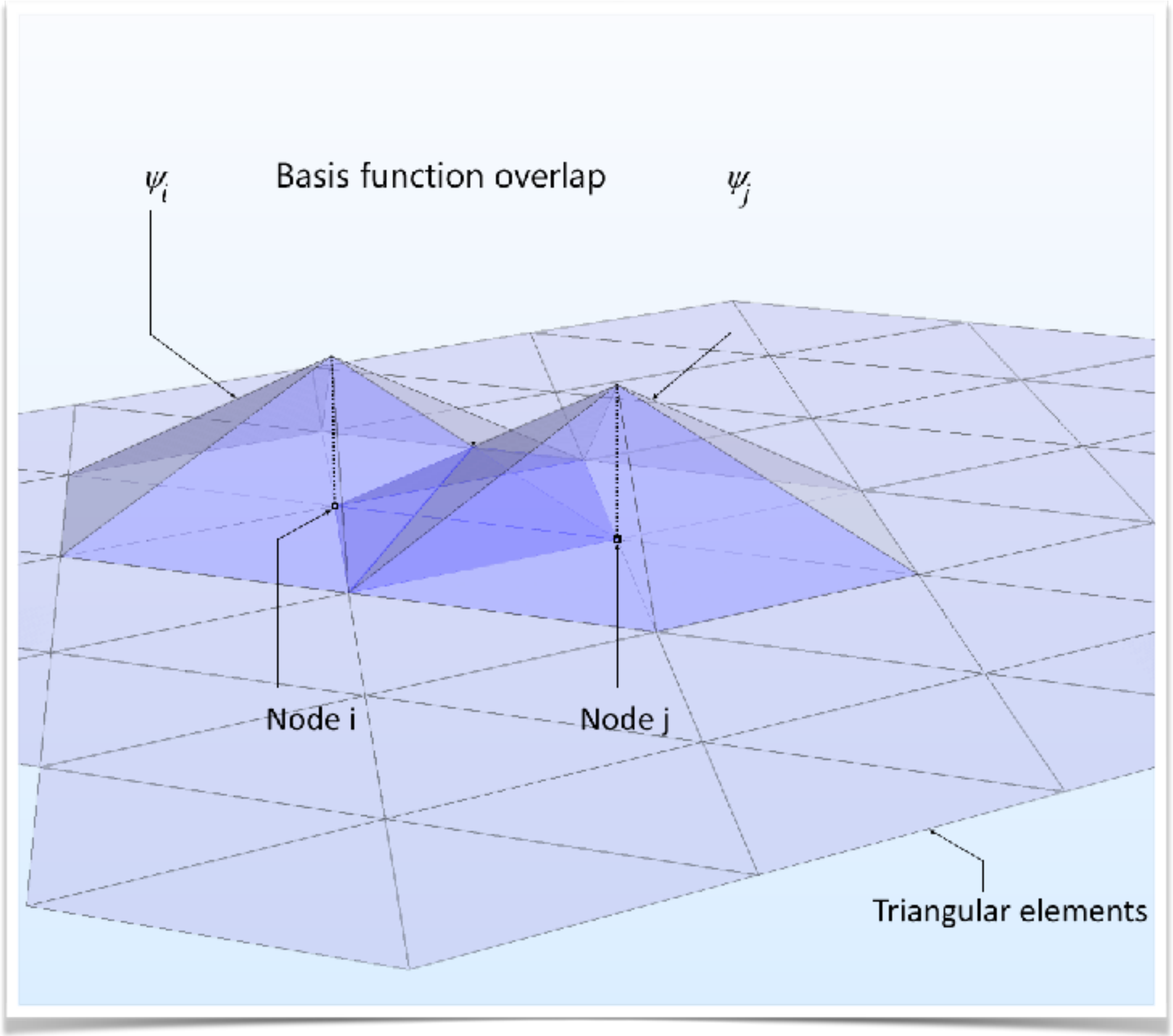
FEM in a nutshell

- Poisson eq: $-\boldsymbol{u}_{xx}-\boldsymbol{u}_{yy}=\boldsymbol{f}$ in Ω s.t. $\boldsymbol{u}=0$ on Γ
- Discretisation by the finite element method:
  - *Basis expansion of the solution*

$$\boldsymbol{u}_h(x,y)=\boldsymbol{u}_1 B_1(x,y)+\ldots+\boldsymbol{u}_n B_n(x,y)$$

Unknown coefficients

User-definable basis functions



Credit: Comsol

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    $$\boldsymbol{u}_h(x,y)=\boldsymbol{u}_1 B_1(x,y)+\ldots+\boldsymbol{u}_n B_n(x,y)$$

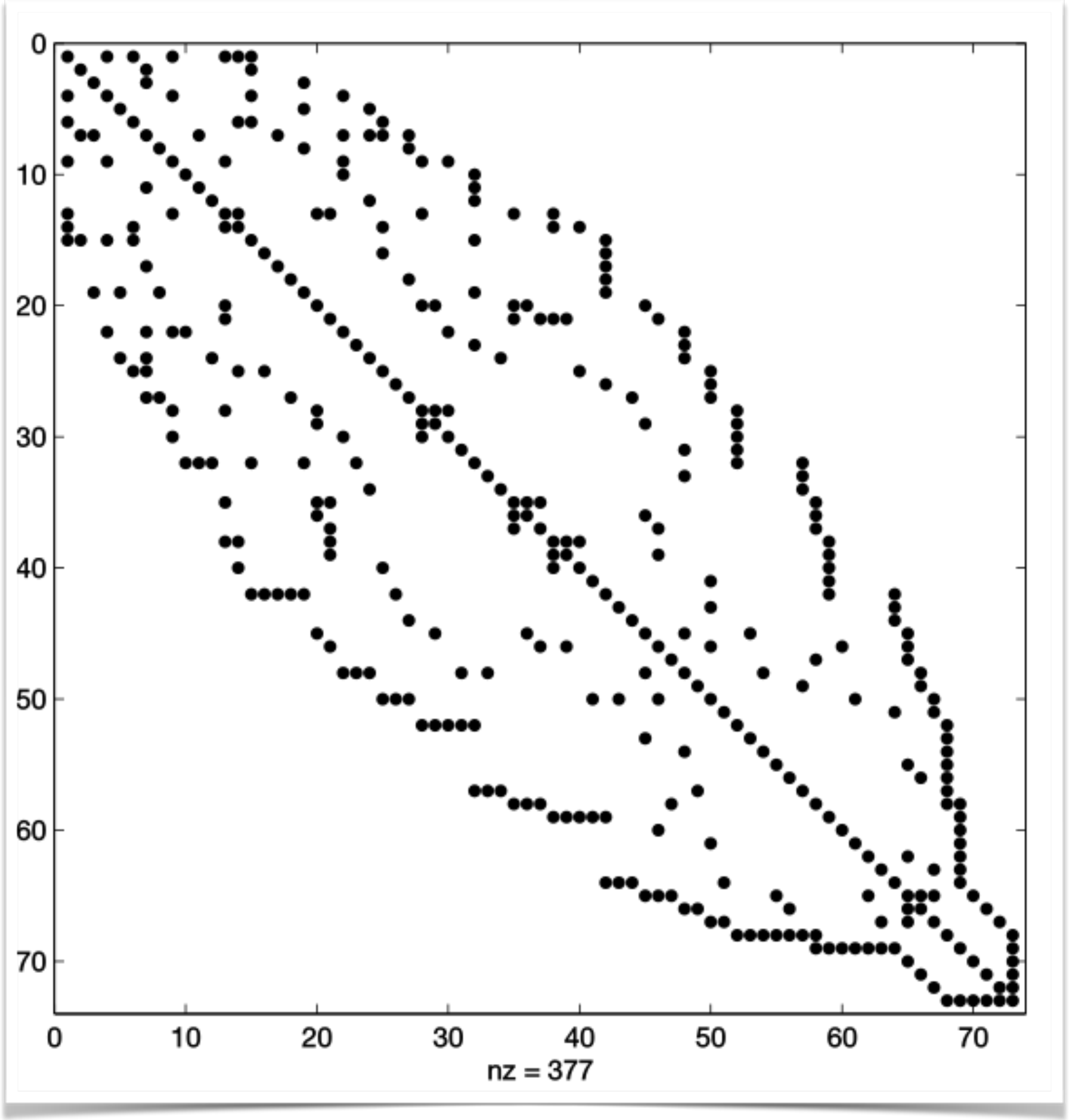
  - *Assembly of stiffness matrix* $\boldsymbol{A}_h$

    $$\boldsymbol{a}_{ij}=\int_\Omega B_{i,x}B_{j,x}+B_{i,y}B_{j,y}\,d\Omega$$

    and right-hand side vector $\boldsymbol{f}_h$

    $$\boldsymbol{f}_i=\int_\Omega B_i\,\boldsymbol{f}(x,y)\,d\Omega$$

Q-accelerated integration (Heinrich 2002)?



Credit: Wikipedia

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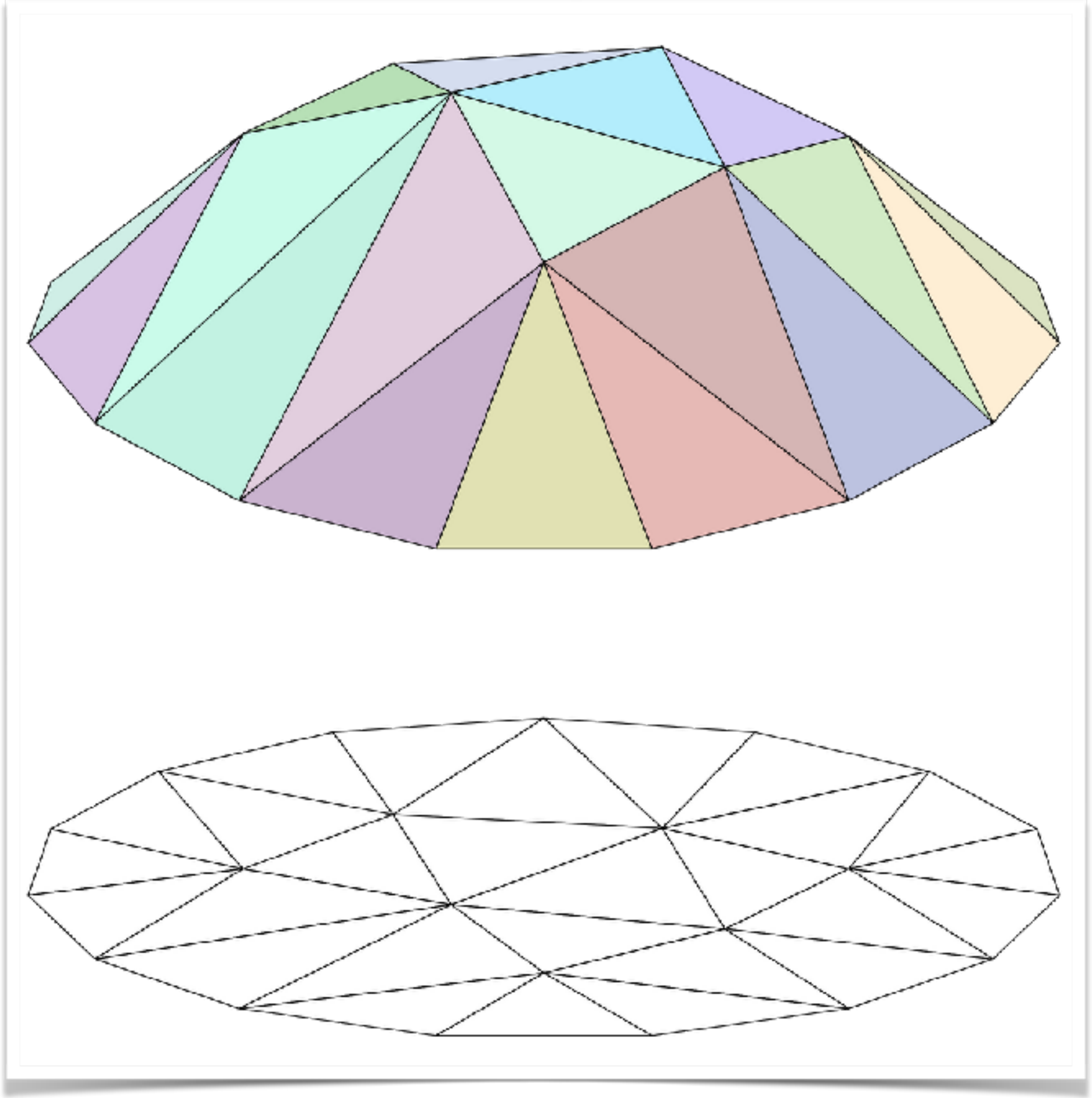
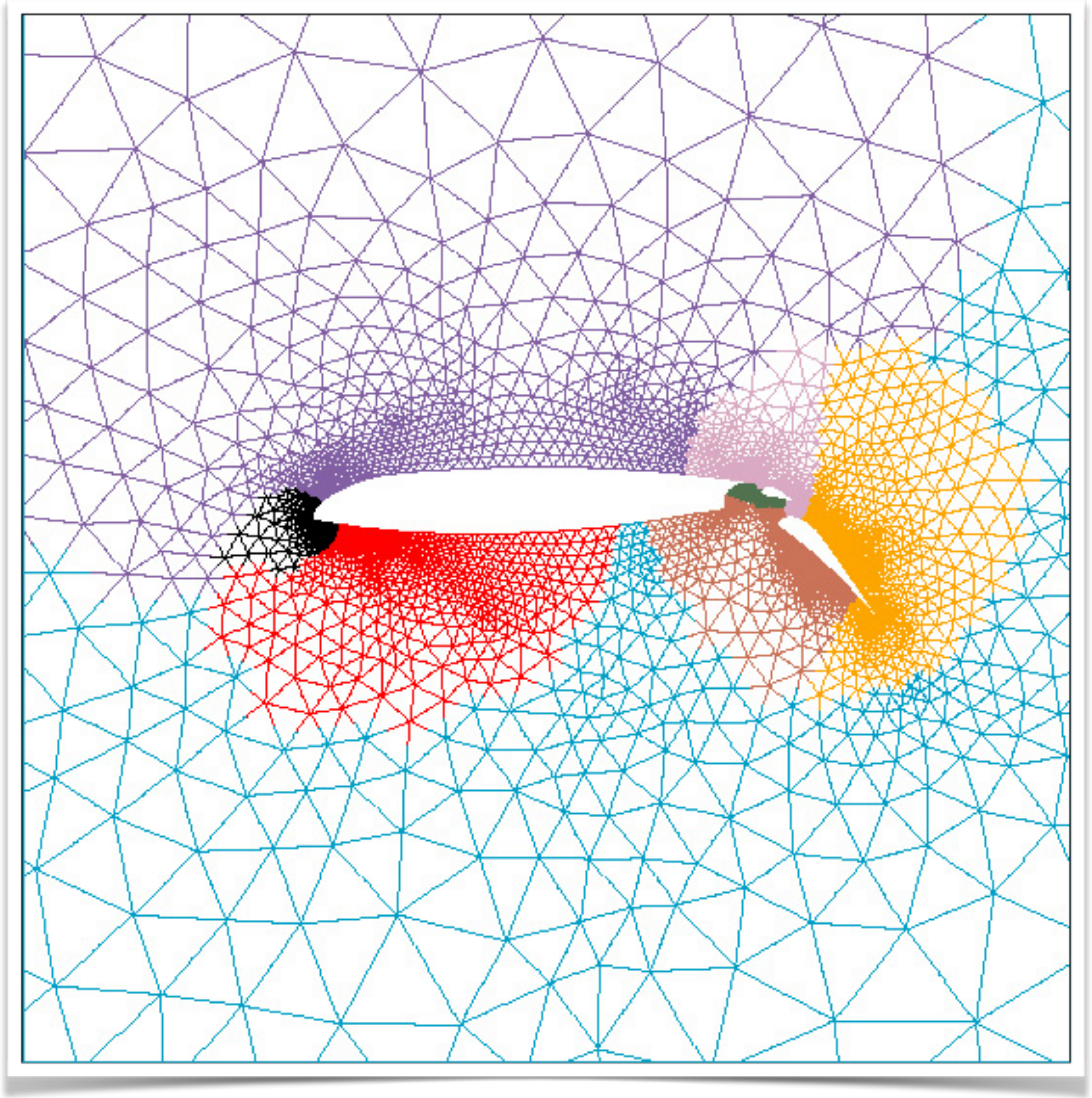
  - *Solution of linear system* $\boldsymbol{A}_h\boldsymbol{u}_h=\boldsymbol{f}_h$

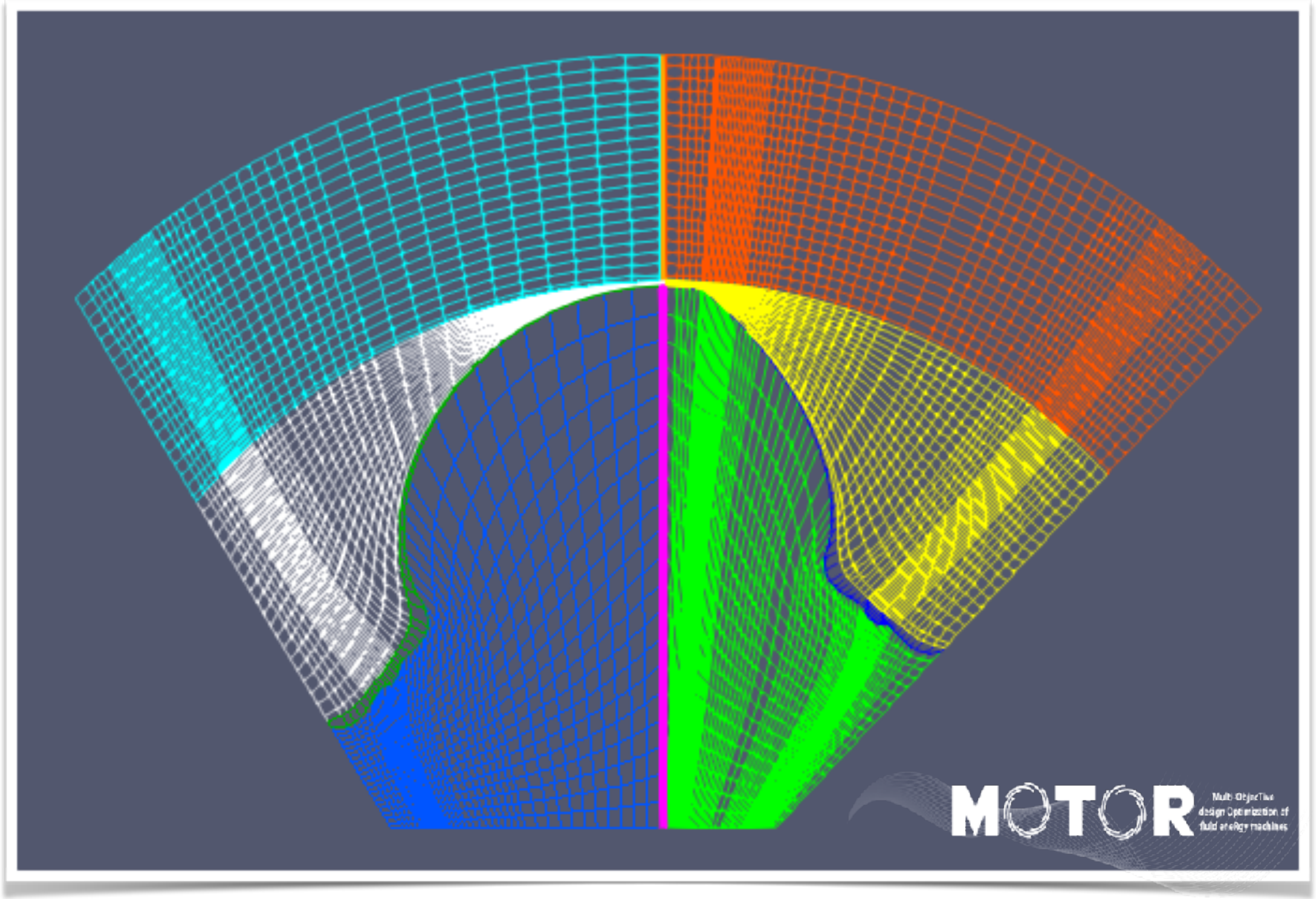


Credit: Wikipedia

Beyond textbook FEM



HPC is a challenge

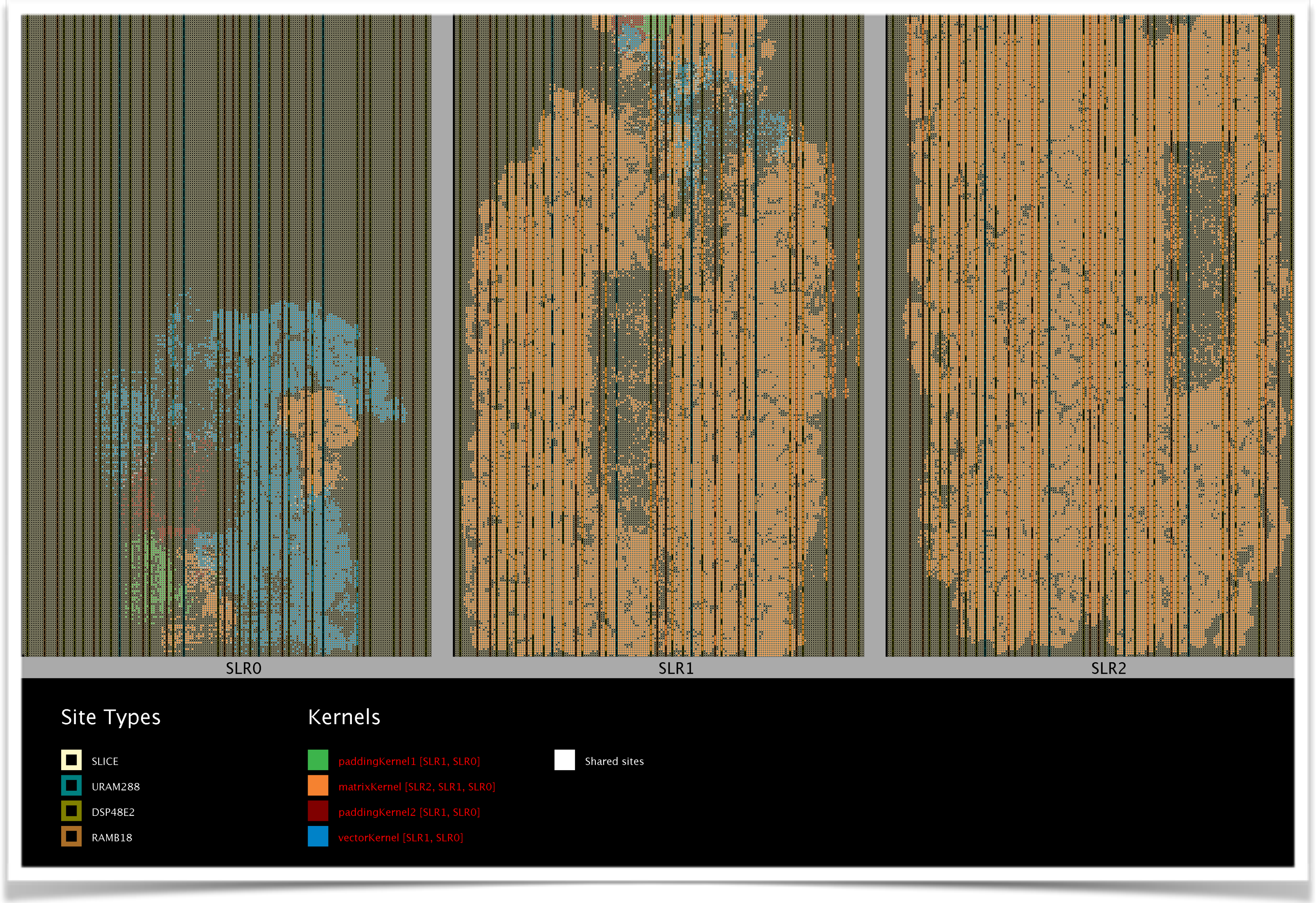


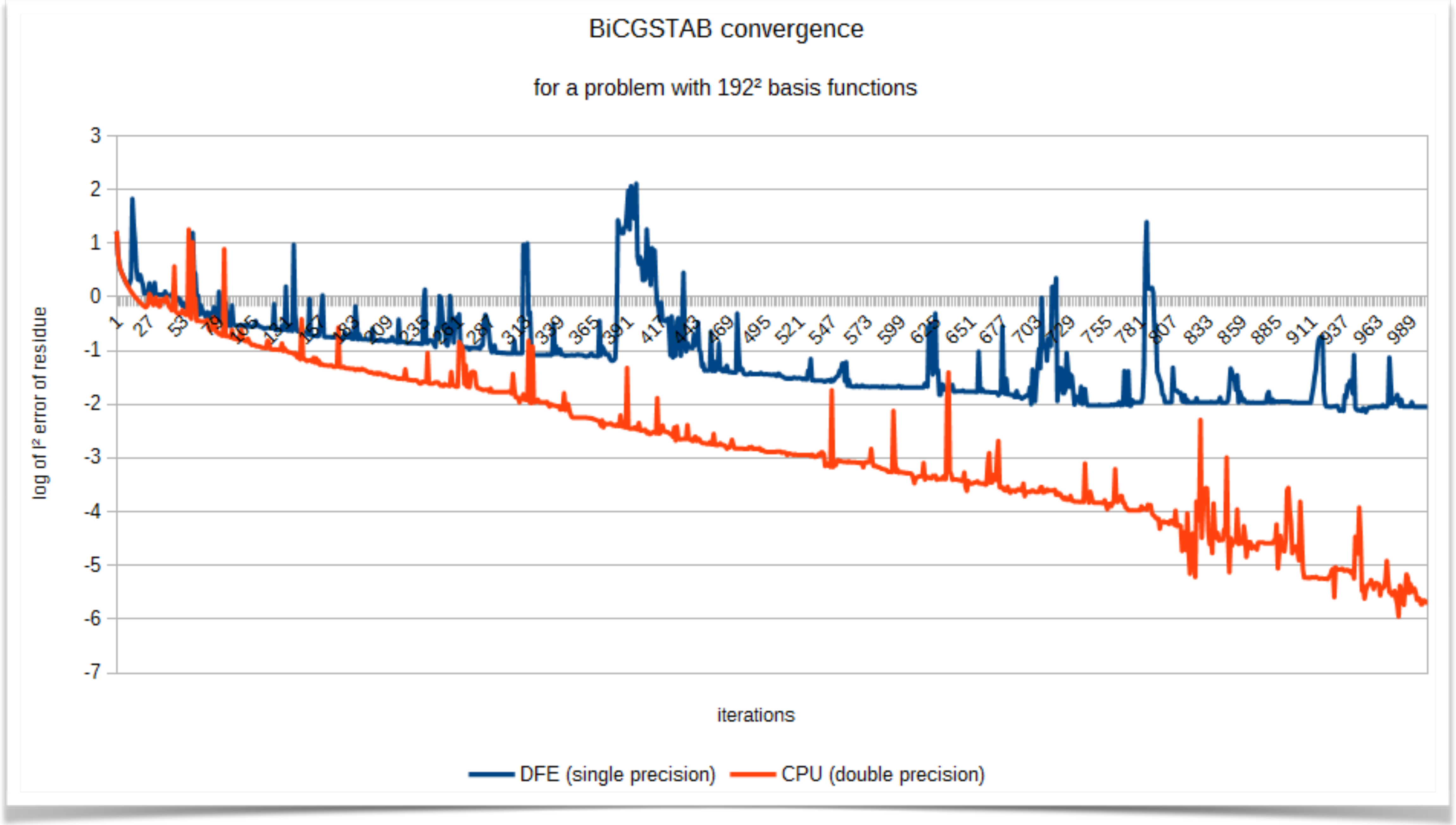
HPC-suitable by design

Credit: J. Hinz, TU Delft

An exotic FEM solver

- Matrix-free solver for quadratic B-Spline basis functions; on-the-fly calculation of matrix coefficients
- MAX4/MAX5 implementations





50 s on CPU @2.0GHz (DP)
10 s on MAX4 @20MHz (SP) <- 5x faster

25-30x faster (projected) on MAX5 with 48bit custom data format for reals

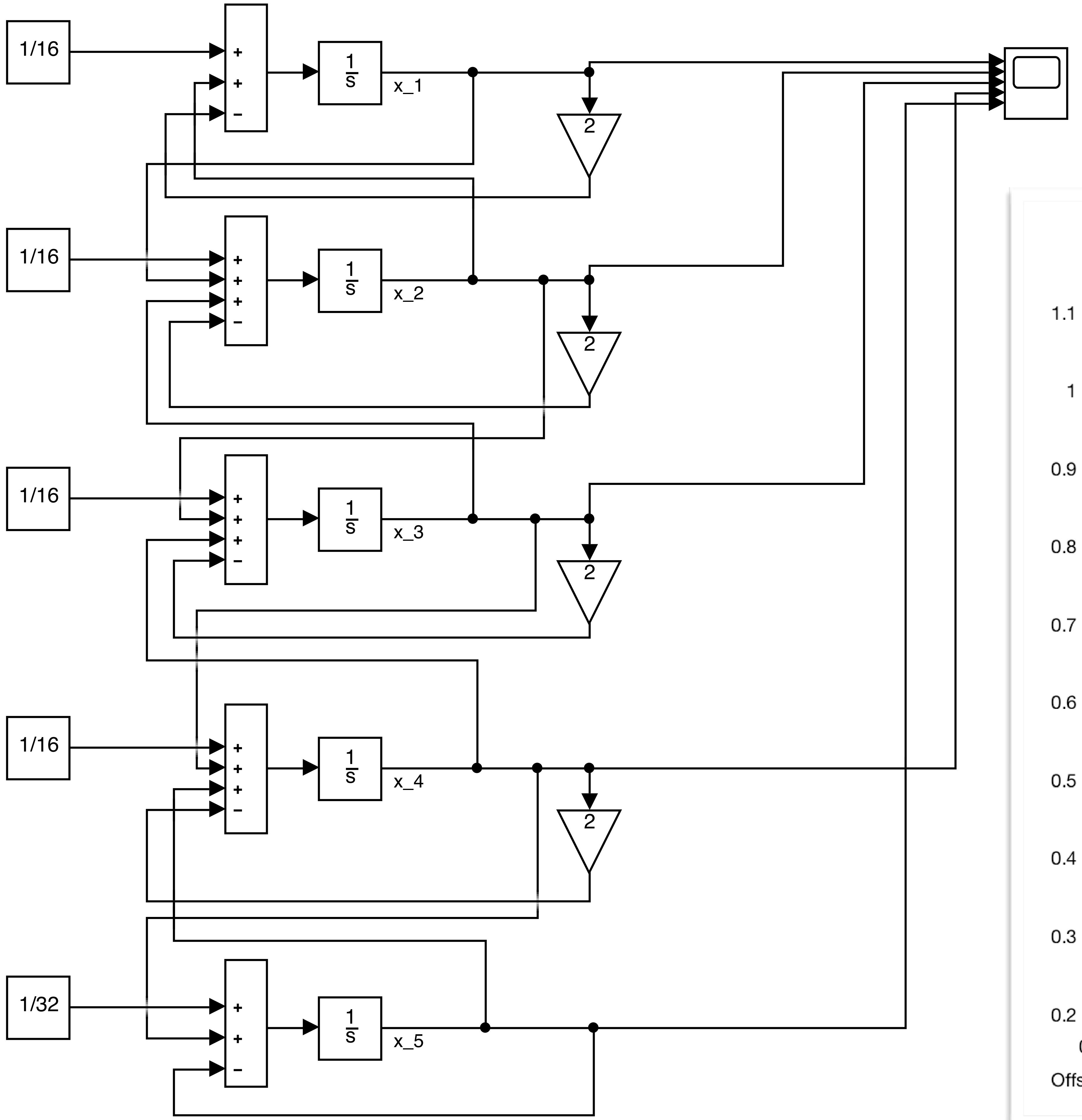
Credit: R. v. Nieuwpoort, TU Delft

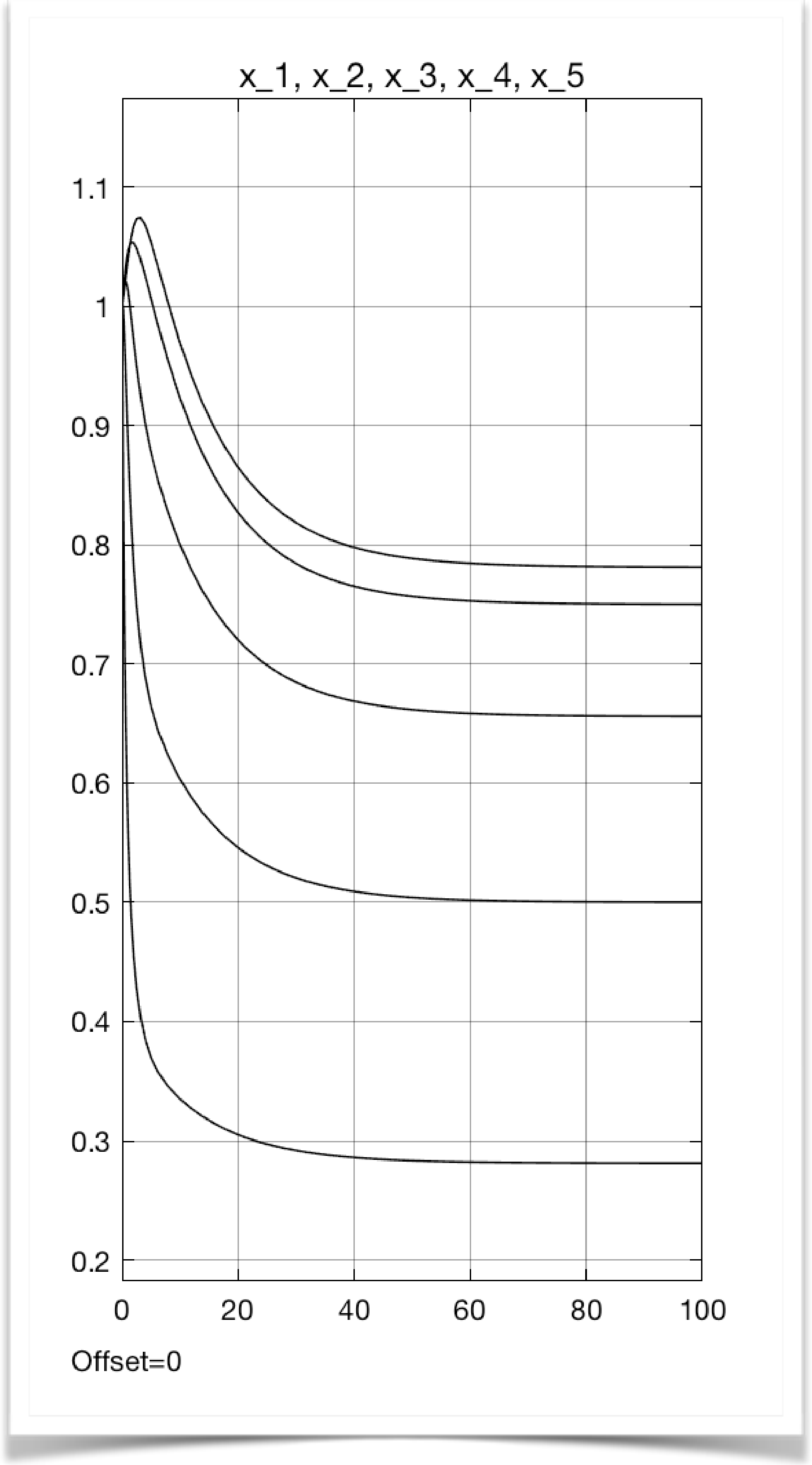
Another exotic FEM solver

- Solution to the linear system $\boldsymbol{A}_h \boldsymbol{u}_h = \boldsymbol{f}_h$ can be interpreted as the steady-state limit of the initial value problem

$$d\boldsymbol{u}_h(t)/dt = \boldsymbol{f}_h - \boldsymbol{A}_h \boldsymbol{u}_h(t),$$
$$\boldsymbol{u}_h(0) = \boldsymbol{u}_0$$

- Acceleration potential using (virtual) analog computing





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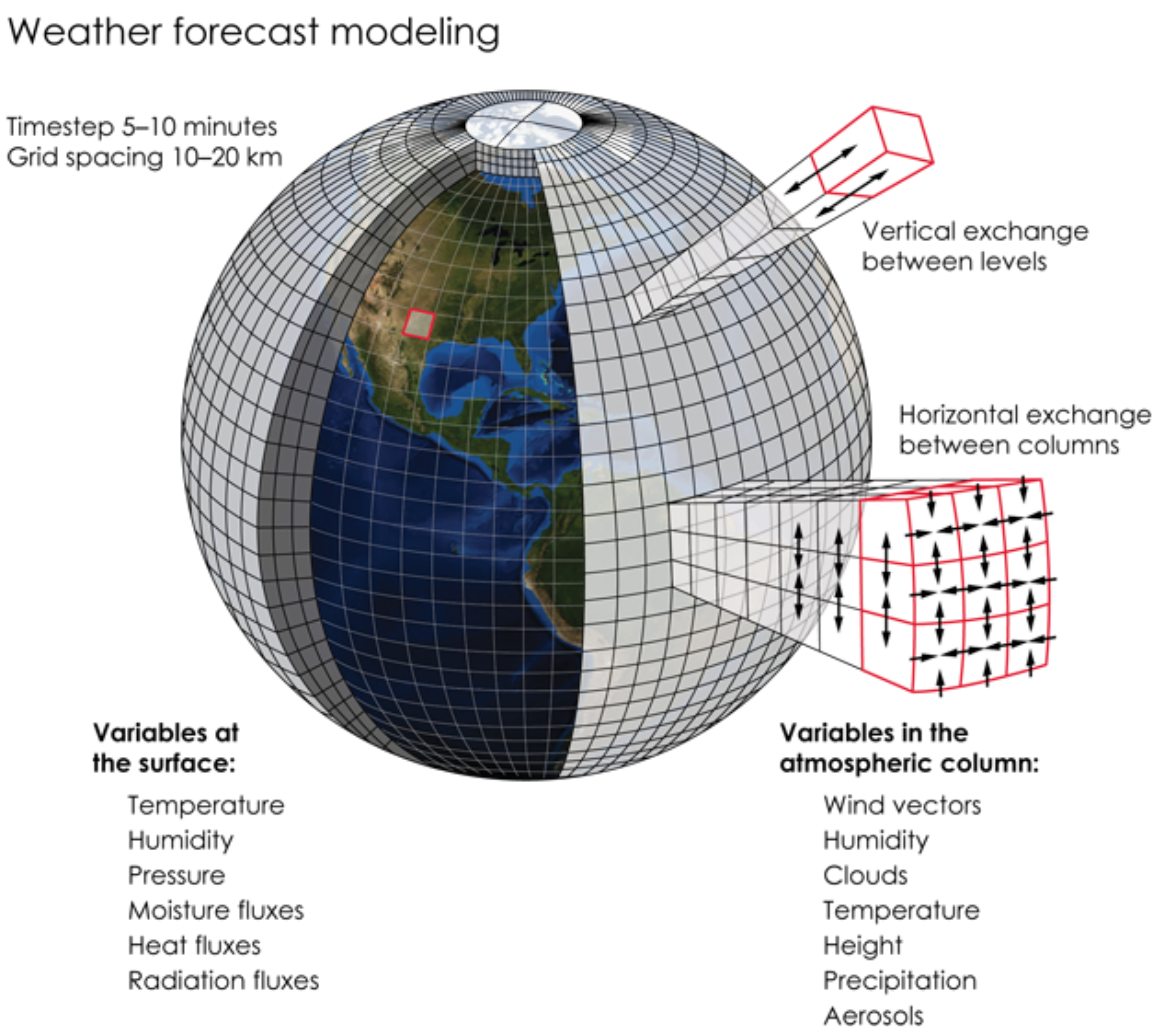
- Acceleration potential using (virtual) analog computing

- Next steps:
  - $(\boldsymbol{A}_h, \boldsymbol{f}_h)/s$—$ts$ value-time scaling to reduce the dynamic range
  - "Assembly" of $\boldsymbol{A}_h, \boldsymbol{f}_h$ via steady state continuous process
  - "Reduction" of $\boldsymbol{u}_h$ into scalar output quantity $J=\boldsymbol{u}_h^T\boldsymbol{M}\boldsymbol{u}_h$
  - Prototype FPGA-implementation
- Inspiration for Q-FEM solver(?)

Quantum Computers

The next step in accelerator technologies?

Simulation-based forecasting



- PDE-based mathematical model: *physical conservation laws*
- Discretisation in space:

  5 million grid points

  x 100 vertical levels

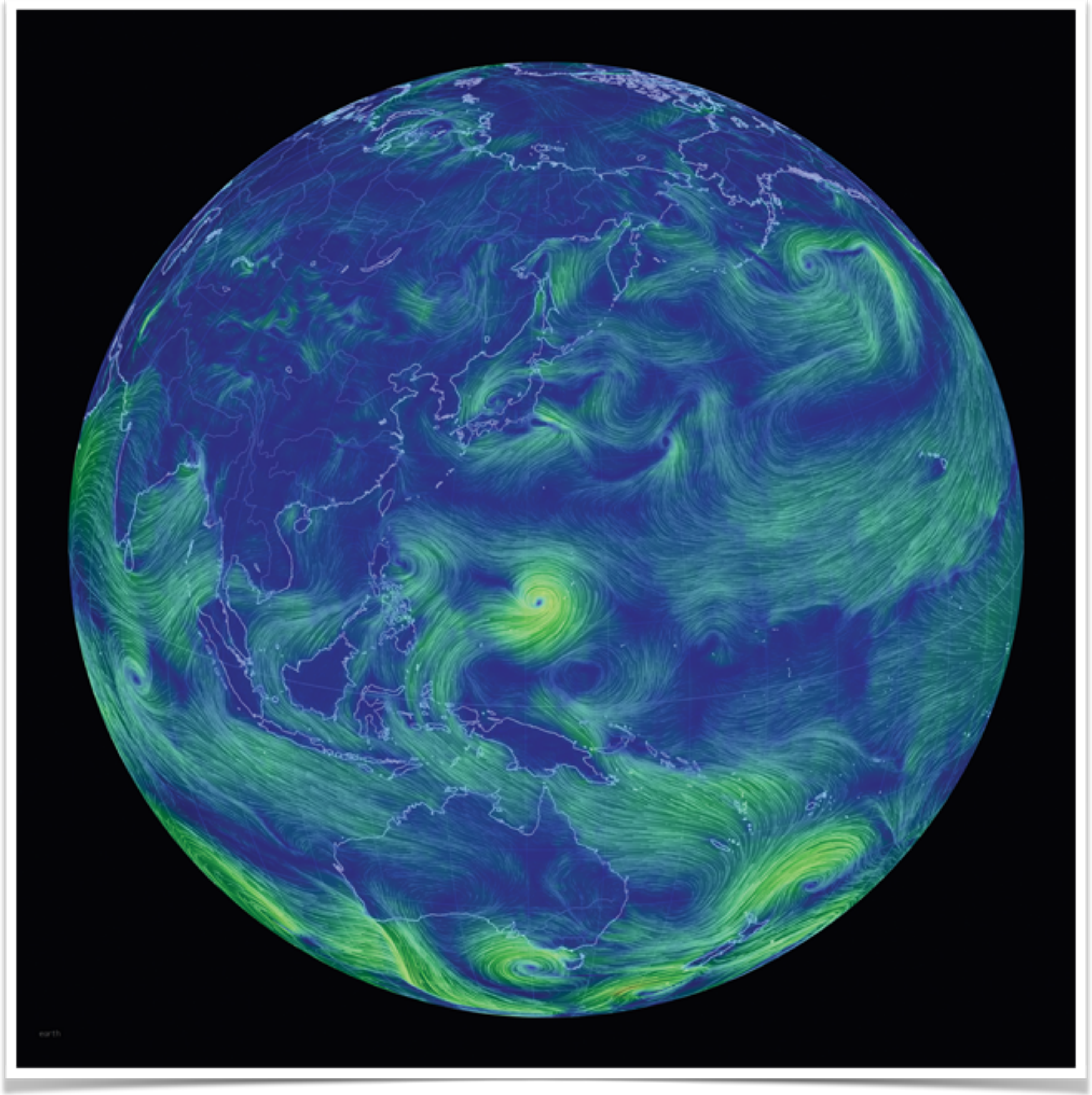
  x 10 prognostic variables

  = 5 billion unknowns in space
- Discretisation in time:

  864 time steps for 72h-forecast

Credit: K. Cantner, AGI

Simulation-based forecasting

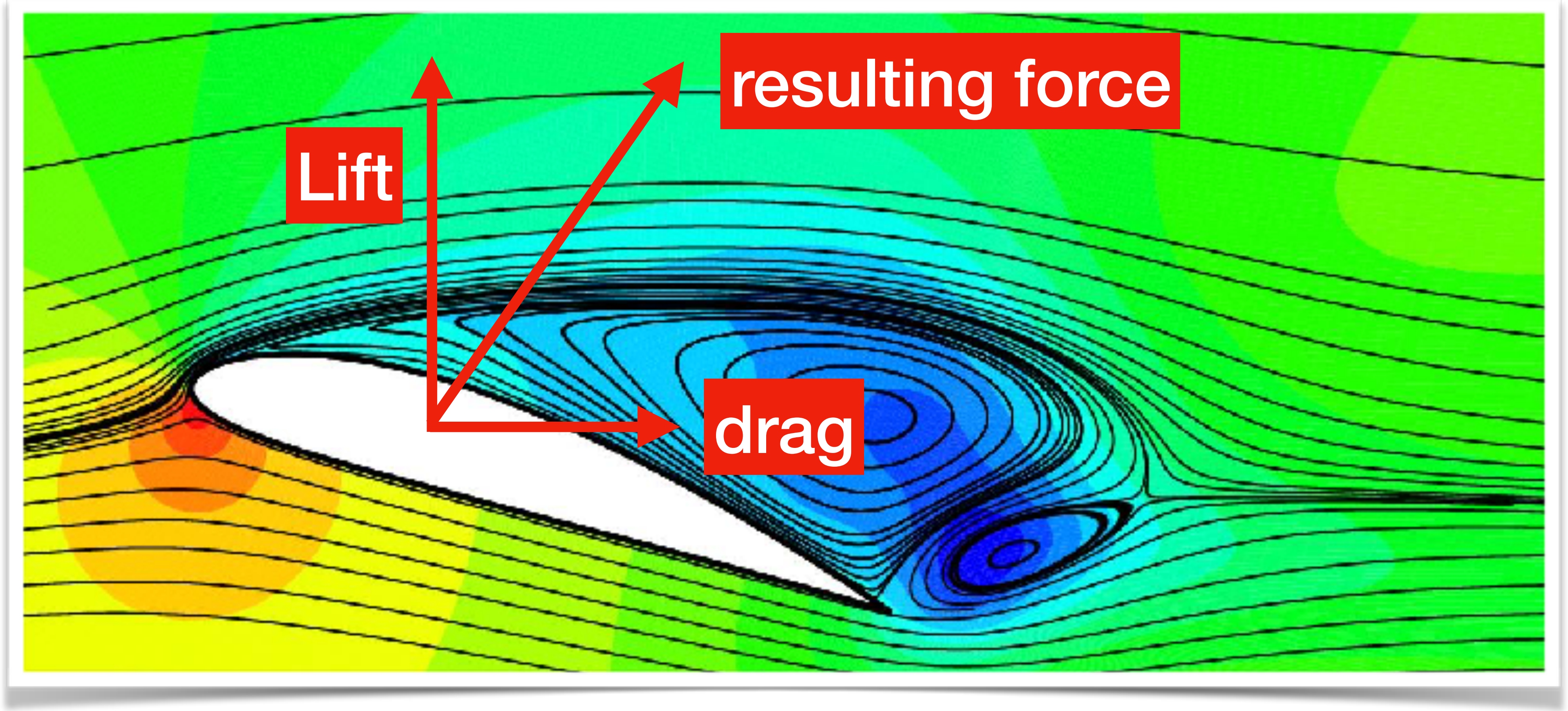


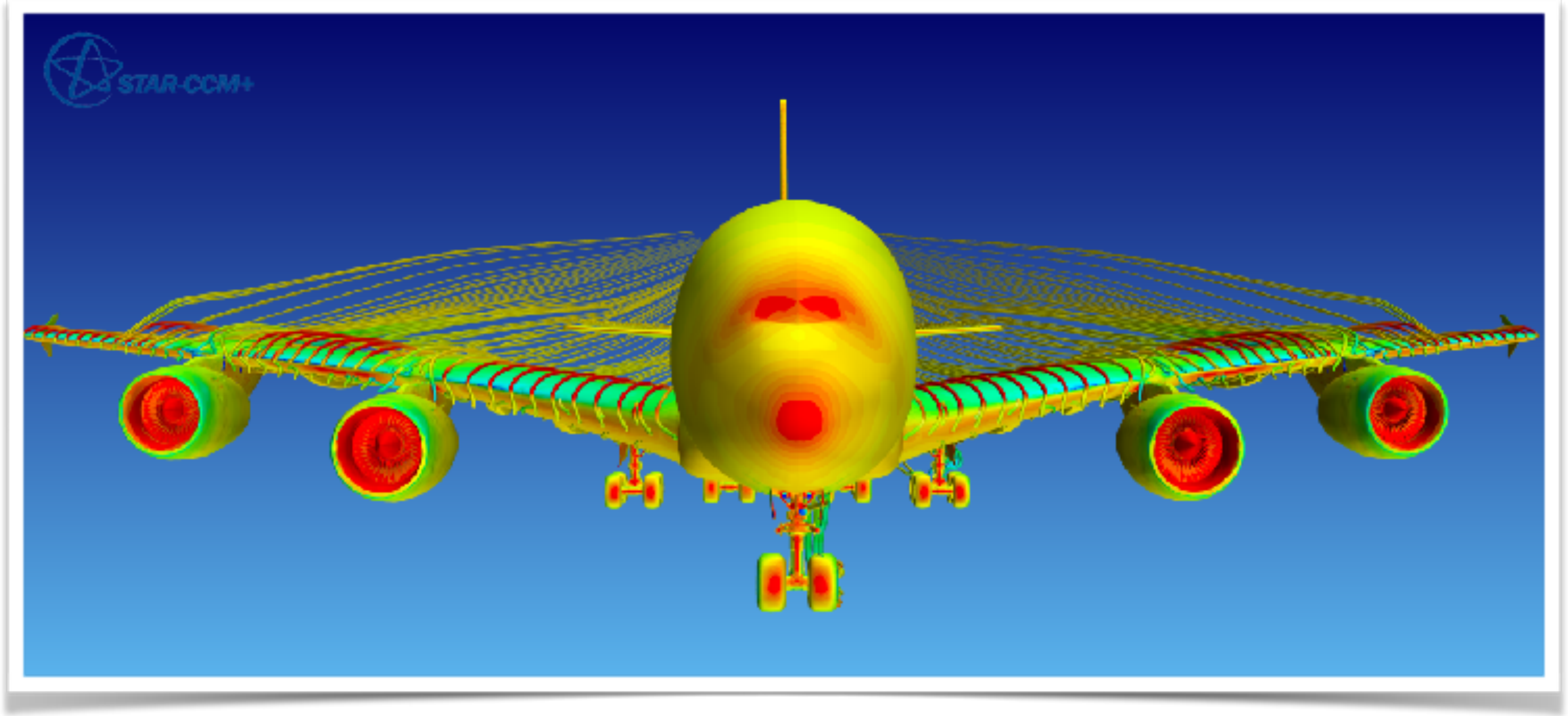
Credit: Cameron Beccario, https://earth.nullschool.net/

- Quantity of interest (QoI):
  Time evolution of field variables
- ECMWF at Reading, UK today:
  simulation of single 10-day forecast in one hour with 10,000 processors
- Future challenges:
  increase model resolution by factor 2,000 (1km, 200 levels, 100 variables) and time-step size to improve forecast accuracy requires 20 million processors!
- Suitable for Q-acceleration:
  no, due to large size of output data

Simulation-based engineering

- QoI: key performance functionals
  "find $J_1(U)$, $J_2(U)$,… such that U solves the discretised problem formulation"
- Example: *cruise L/D (higher is better)*
  B747-200 (1969): 15.3
  B777-200 (1994): 19.3
- Future challenges:
  increase model resolution and complexity; turbulence modelling; CAD integration; virtual twins for lifetime analysis
- Suitable for Q-acceleration:
  maybe, since it fits into QLSA setup but the problem sizes might be too large

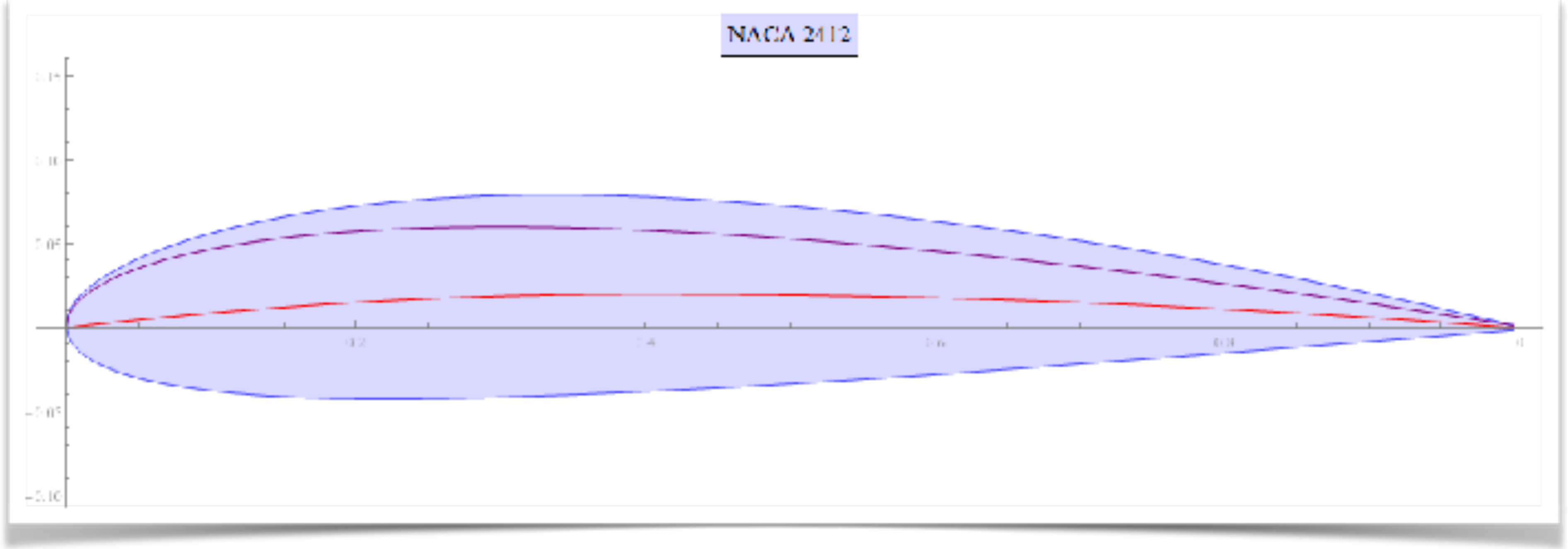


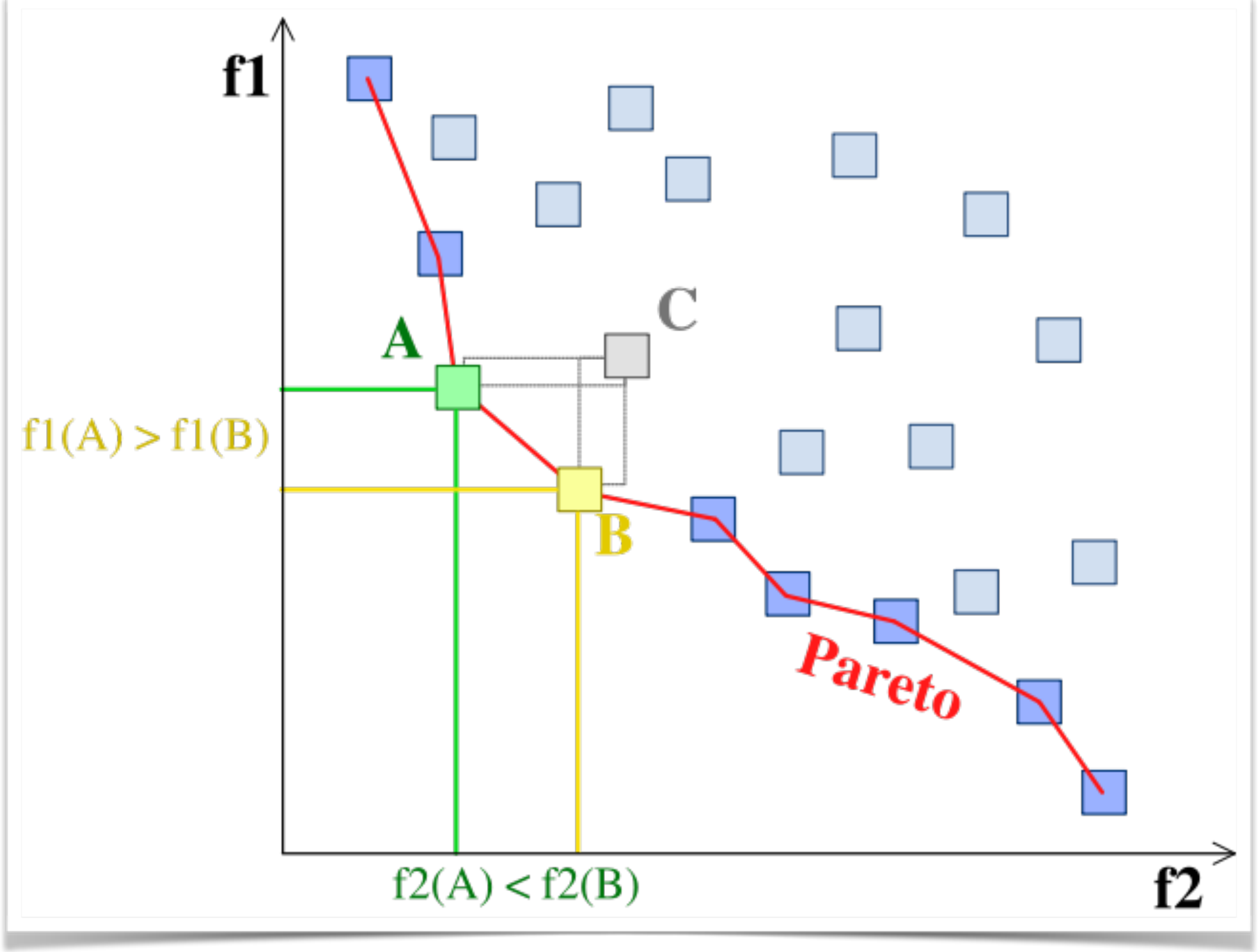


Credit: Siemens

Simulation-based optimisation

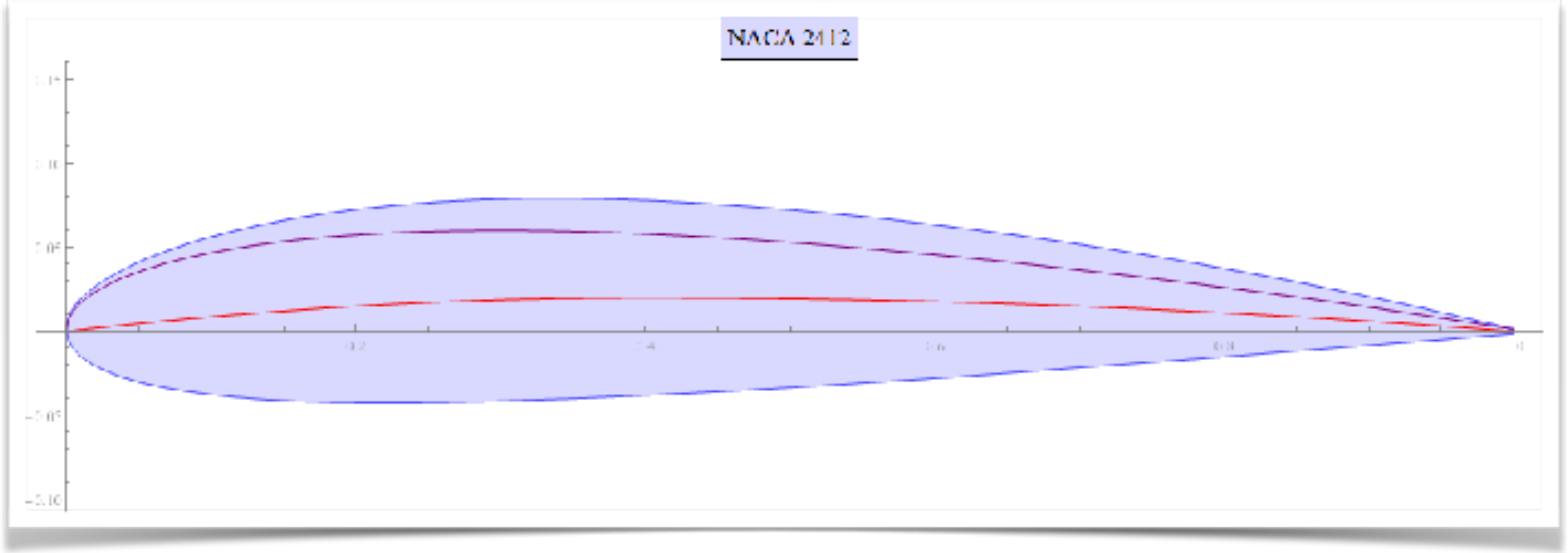
- Input: *design parameters p_1, p_2,… controlling the shape of the wing*
- QoI: *Pareto front of optimal design parameters* $\mathbf{p}^*$ *such that the solutions* $U(\mathbf{p}^*)$ *to the discretised PDE problems maximise ‘all’ key performance functionals f1, f2,…*
- Solution approaches: $\mathbf{p}^k \rightarrow \mathbf{p}^{k+1}$
    - *Gradient-free methods:* evolution-inspired algorithms for generating populations of parameters
    - *Gradient-based methods:* choose parameters ‘in the direction’ that brings $U(\mathbf{p}^{k+1})$ closer to an optimal state

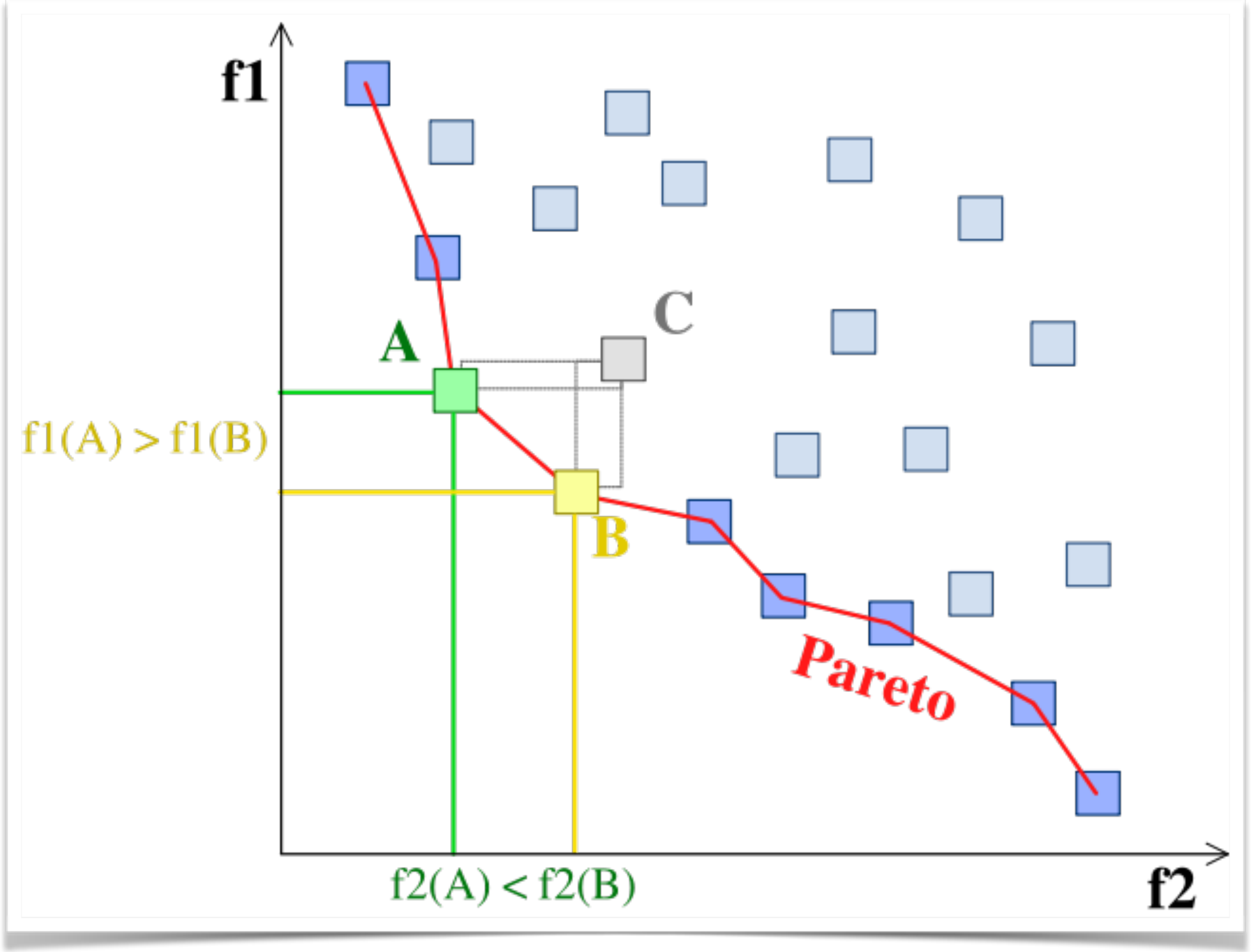




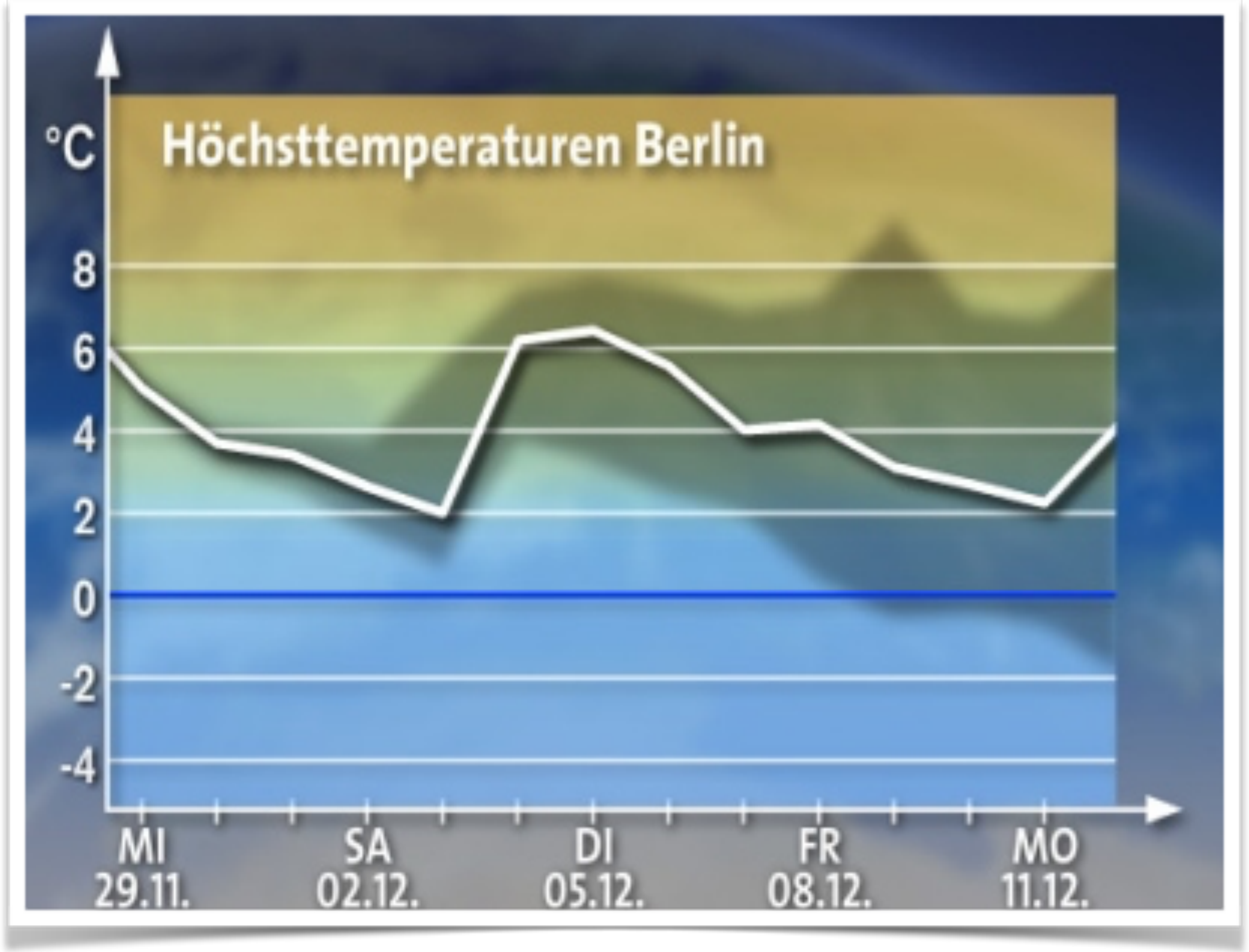
Simulation-based optimisation

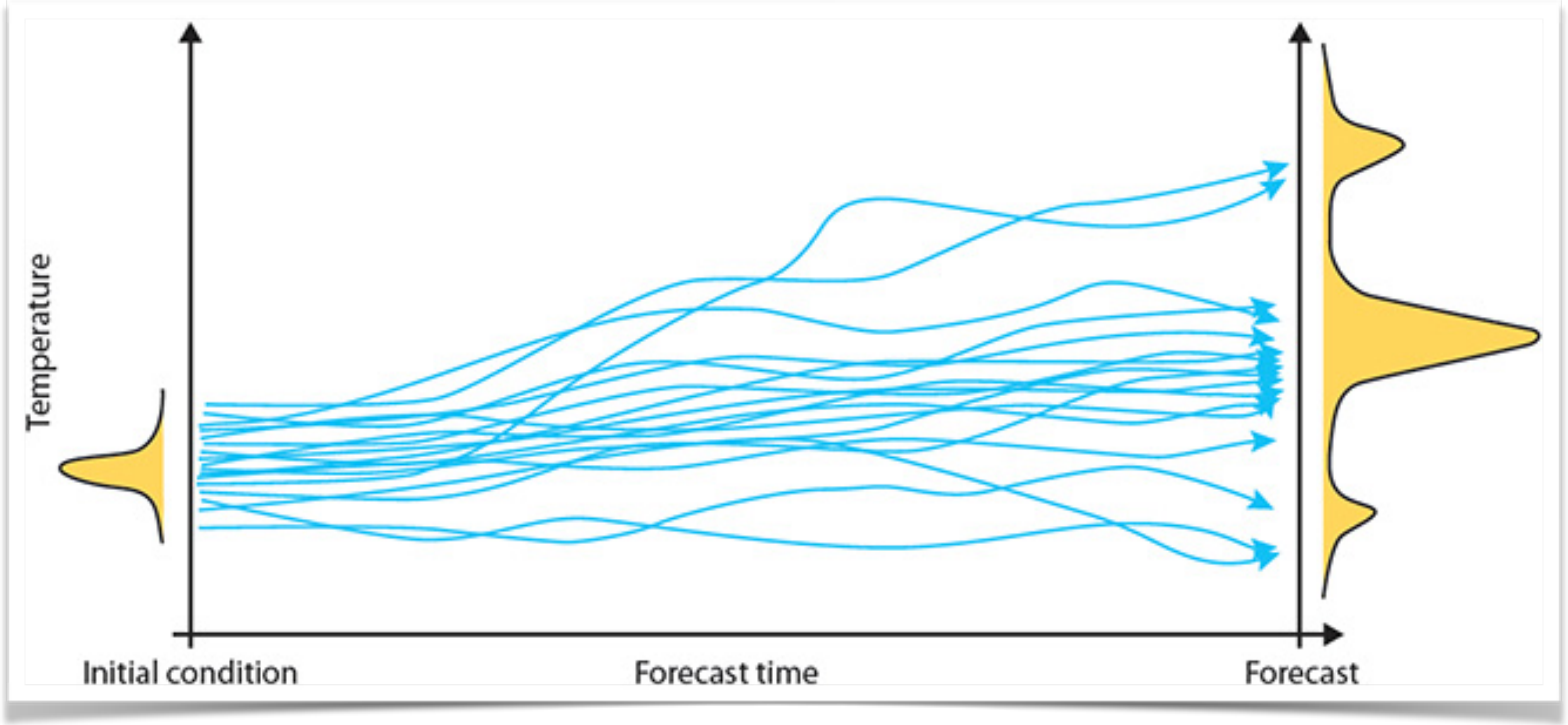
- Future challenges:
  “curse of dimensionality”; efficient exploration of entire design space
- Suitable for Q-acceleration:
  maybe, since efficient quantum algorithms for gradient estimation and quantum-based optimisation exist, however, mainly for discrete optimisation problems





Uncertainty quantification





Credit: ECMWF

- Ensemble forecasting: *Monte-Carlo analysis accounting for uncertainties in initial conditions, mathematical model, data etcetera*
- QoI: *range of possible scenarios (in terms of target functionals) and their likelihood of occurrence*
- Suitable for Q-acceleration: *maybe, since QC requires multiple simulation runs anyway but the problem sizes might be too large*

Quantum linear solvers

- QLSA: HHL ’08, Ambainis ’10, Clader et al. ’13, Childs et al. ’15, Kerenidis ‘17
- Input:
  - *NxN s*-sparse Hermitian matrix ***A*** with condition number $\varkappa = \|A\| \, \|A^{-1}\|$ and eigenvalues $1/\varkappa \leqq |\lambda_i| \leqq 1$, and a right-hand side unit vector ***f***
- Output:
  - Scalar QoI $J(\mathbf{u}) = \mathbf{u}^T \mathbf{M} \mathbf{u}$ (***M*** is a matrix) such that ***u*** solves $\mathbf{A}\mathbf{u} = \mathbf{f}$
- Complexity:
  - Best classical algorithm $O(\varkappa^{1/2} N)$
  - Quantum algorithms $O(\varkappa \log^3 \varkappa \log N)$—$O(\varkappa^2 \log N)$ ⬅ exponential speed-up

Q-FEM solver for Poisson’s equation

- $\boldsymbol{A}_h$ is s.p.d., *s*-sparse, well-conditioned ✓
- $\boldsymbol{f}_h$ is unit vector (after dynamic range scaling) ✓
- Matrix entries in row are accessible in time *O(s)* ✓
- Efficient ‘preparation’ of right-hand side quantum state (✓)

- Can we compute $||\boldsymbol{u}_h||^2 = \boldsymbol{u}_h^T \boldsymbol{u}_h$ where $\boldsymbol{u}_h$ solves Poisson’s equation?

Q-FEM solver for Poisson’s equation

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Quantum algorithms and the finite element method

Ashley Montanaro and Sam Pallister*
School of Mathematics, University of Bristol, Bristol BS8 1TW, United Kingdom
(Received 5 January 2016; published 17 March 2016)

- *“when one compares quantum and classical algorithms for the FEM fairly by considering every aspect of the problem – including the complexity of producing an accurate approximation of the desired classical output – an apparent exponential quantum advantage can sometimes disappear”*
- *“there are still two types of problem where quantum algorithms for the FEM could achieve a significant advantage over classical algorithms: those where the solution has large higher-order derivatives, and those where the spatial dimension is large”*

Q-accelerated scientific computing

- **Challenges**
  - Sufficient #qubits for realistic problem sizes
  - Q-system hw/sw infrastructure, error correction
- **Open problems**
  - Real numbers (IEEE-754, continuous encoding, custom formats)
  - Divide-and-conquer/domain decomposition (no-cloning principle!)
  - Validation of results (using classical supercomputers?)
  - Reproducibility of simulations (but that’s a problem in HPC as well)

Let’s get ready for Q-accelerated scientific computing and exchange ideas both ways!

Thank you for your attention!