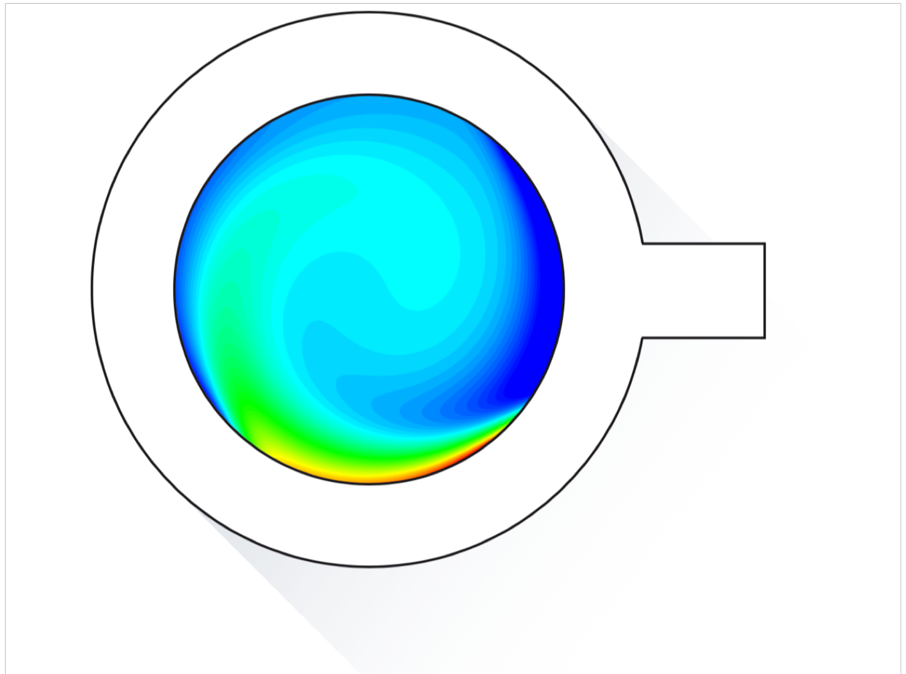


Supercomputing and numerical modelling

Parallel algorithms research lab

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

Hardware

Introduction

TOP 500
The List.

PRESENTED BY

ICL INNOVATIVE COMPUTING LABORATORY

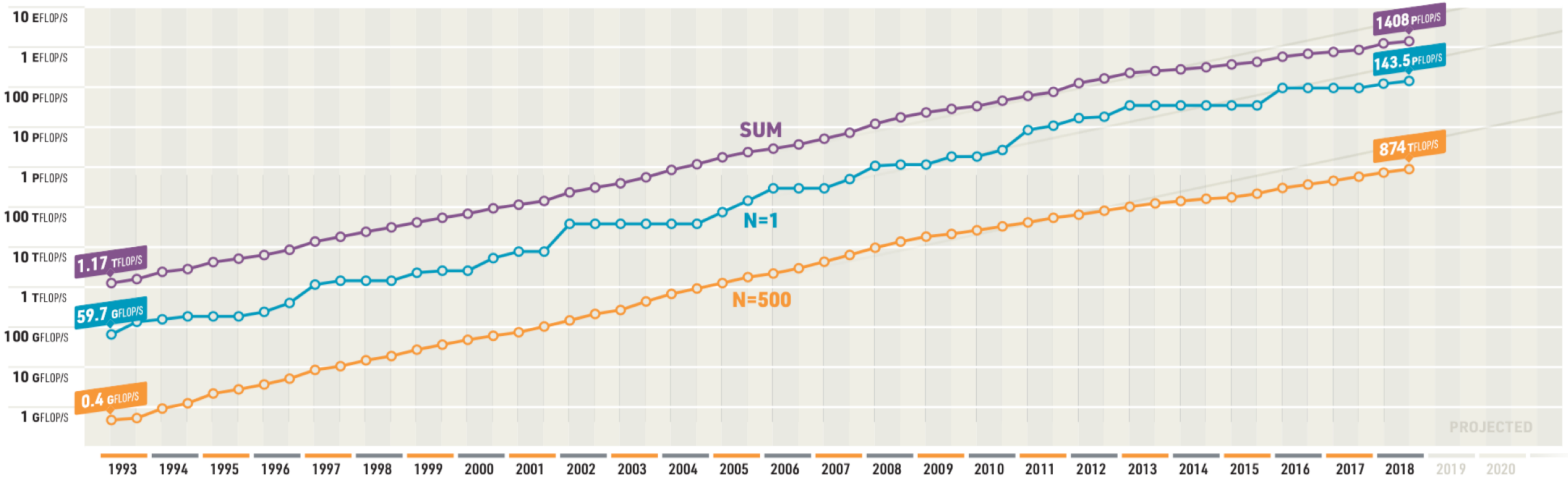
BERKELEY LAB Lawrence Berkeley National Laboratory

ISC GROUP Moving Forward.

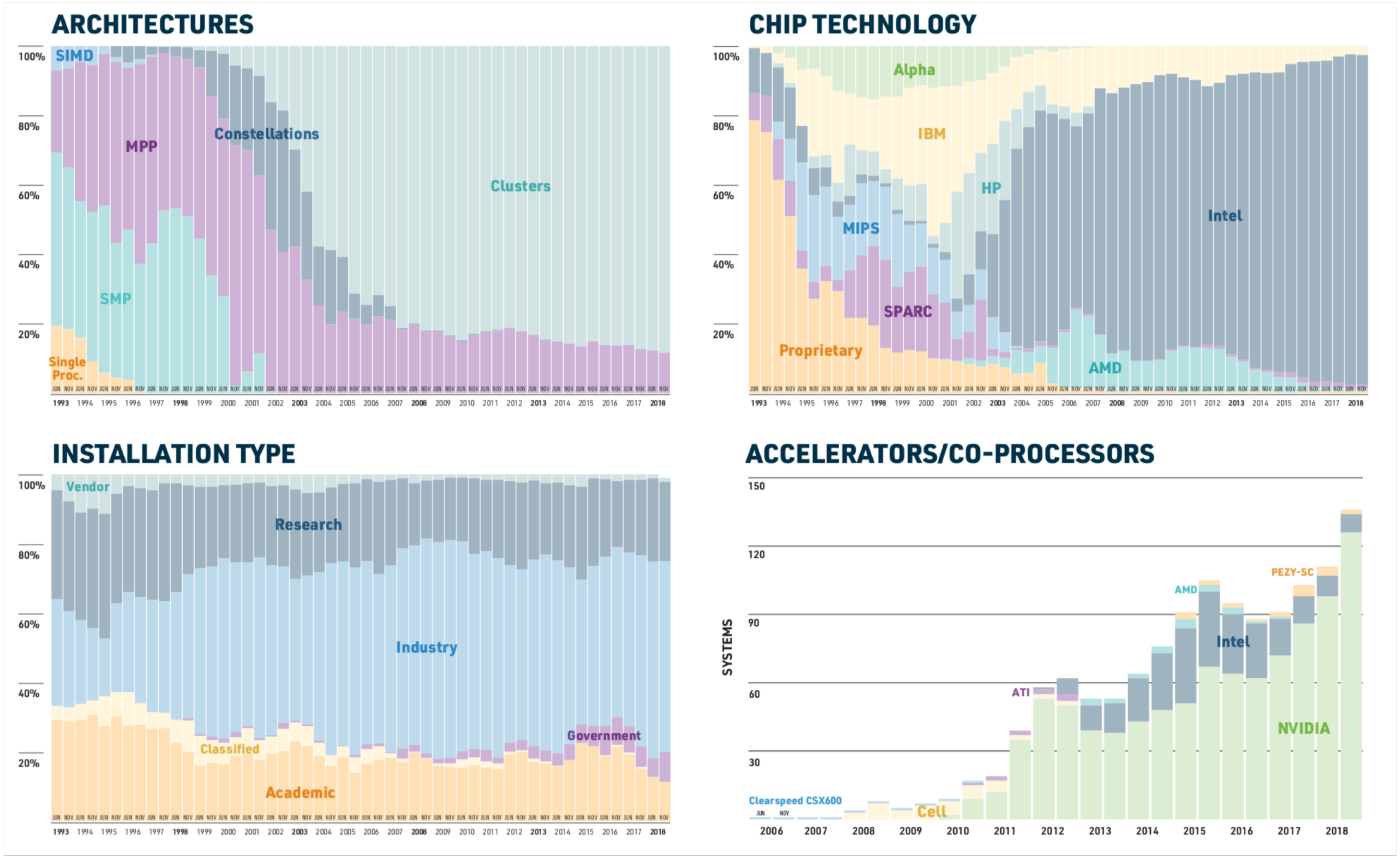
FIND OUT MORE AT top500.org

		SPECS	SITE	COUNTRY	CORES	RMAX PFLOP/S	POWER MW
1	Summit	IBM POWER9 (22C, 3.07GHz), NVIDIA Volta GV100 (80C), Dual-rail Mellanox EDR Infiniband	DOE/SC/ORNL	USA	2,282,544	143.5	11.1
2	Sierra	IBM POWER9 (22C, 3.1GHz), NVIDIA Tesla V100 (80C), Dual-rail Mellanox EDR Infiniband	DOE/NNSA/LLNL	USA	1,572,480	94.6	7.44
3	Sunway TaihuLight	Shenwei SW26010 (260C 1.45 GHz) Custom interconnect	NSCC in Wuxi	China	10,649,600	93.0	15.4
4	Tianhe-2A (Milkyway-2A)	Intel Ivy Bridge (12C 2.2 GHz) & TH Express-2, Matrix-2000	NSCC Guangzhou	China	4,981,760	61.4	18.5
5	Piz Daint	Cray XC50, Xeon E5-2690v3 (12C 2.6GHz), Aries interconnect , NVIDIA Tesla P100	CSCS	Switzerland	319,424	21.2	2.38

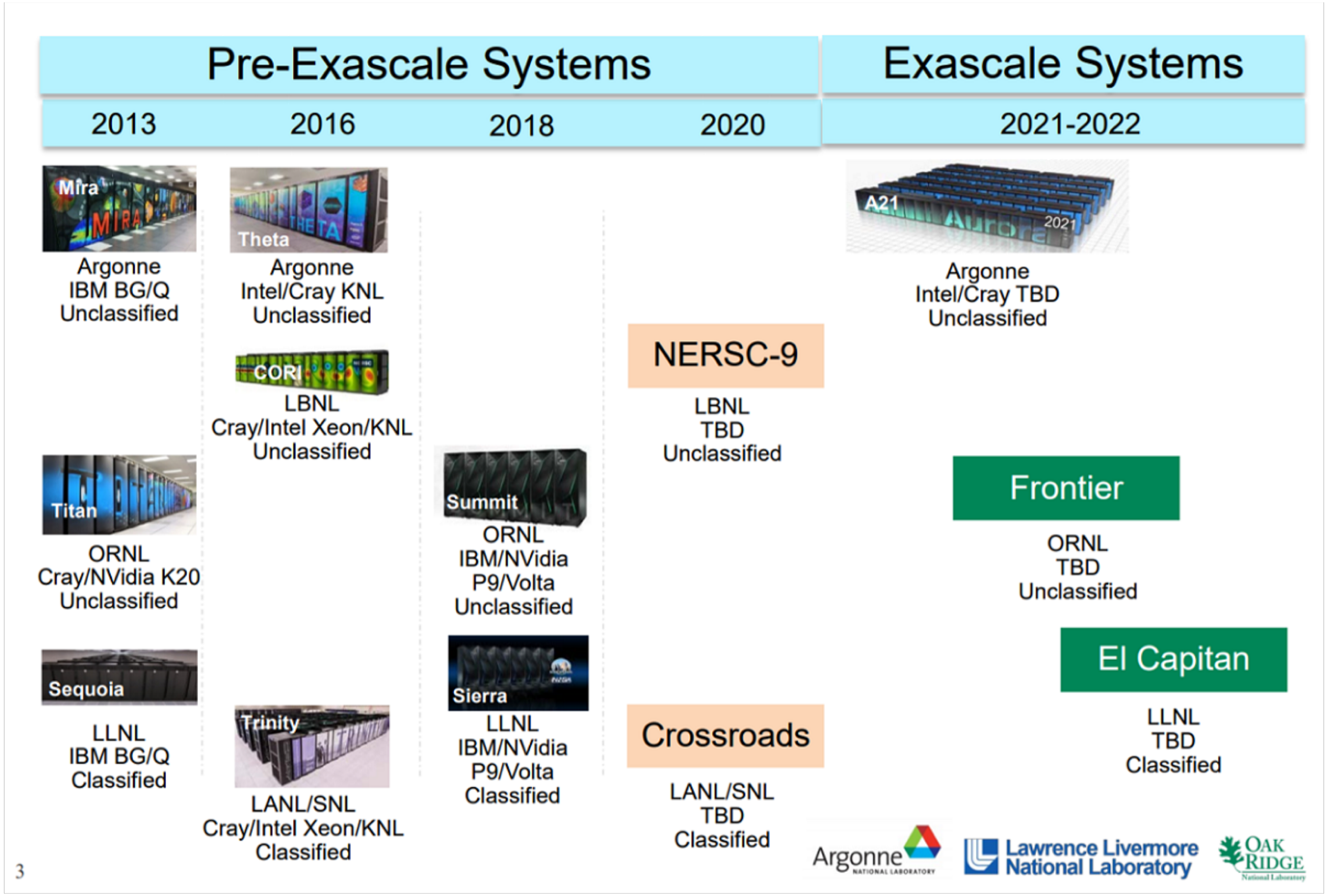
PERFORMANCE DEVELOPMENT



Introduction

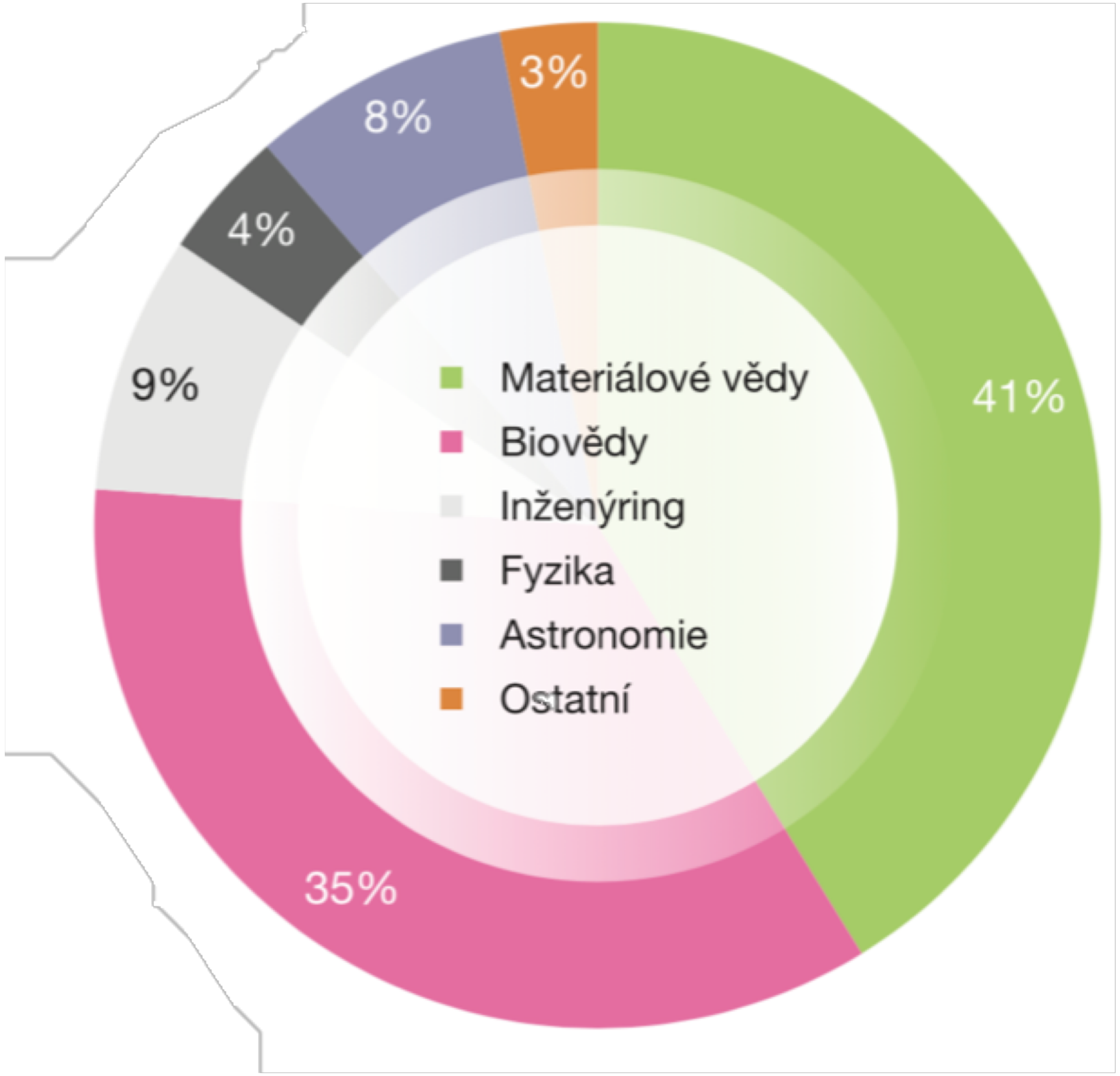


Next-generation U.S. Department of energy supercomputers



Introduction

A single Apple iPhone 5 has 2.7 times the processing power than the 1985 Cray-2 supercomputer.



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8%
4%
9%
41%
35%
Materiálové vědy
Biovědy
Inženýring
Fyzika
Astronomie
Ostatní

Virtual Prototyping


FKFS

Fluid Flow - Navier-Stokes equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} &= 0 && (1)\\
\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2)}{\partial x} + \frac{\partial (\rho u v)}{\partial y} + \frac{\partial (\rho u w)}{\partial z} &= -\frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) && (2)\\
\frac{\partial \rho v}{\partial t} + \frac{\partial (\rho u v)}{\partial x} + \frac{\partial (\rho v^2)}{\partial y} + \frac{\partial (\rho v w)}{\partial z} &= -\frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) && (3)\\
\frac{\partial \rho w}{\partial t} + \frac{\partial (\rho u w)}{\partial x} + \frac{\partial (\rho v w)}{\partial y} + \frac{\partial (\rho w^2)}{\partial z} &= -\frac{\partial p}{\partial z} + \nu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) && (4)\\
\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho u E)}{\partial x} + \frac{\partial (\rho v E)}{\partial y} + \frac{\partial (\rho w E)}{\partial z} &= -\frac{\partial p u}{\partial x} - \frac{\partial p v}{\partial y} - \frac{\partial p w}{\partial z} + S && (5)
\end{aligned}
$$

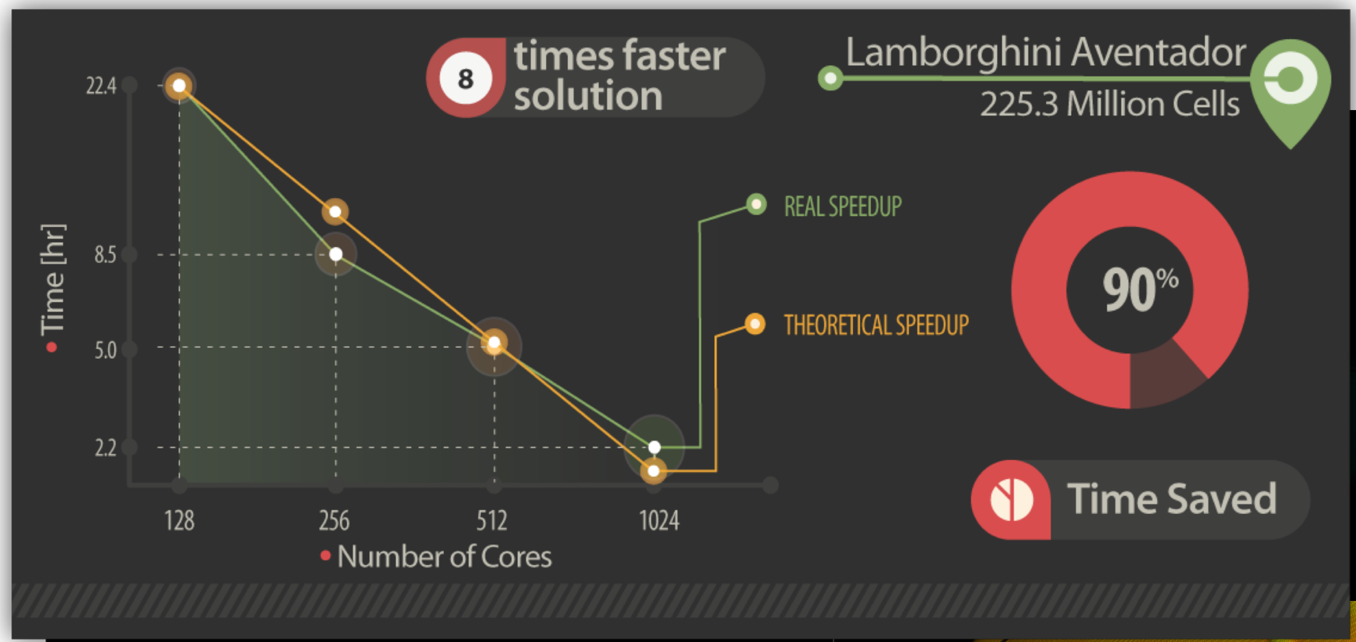
Millennium Prize Problem:

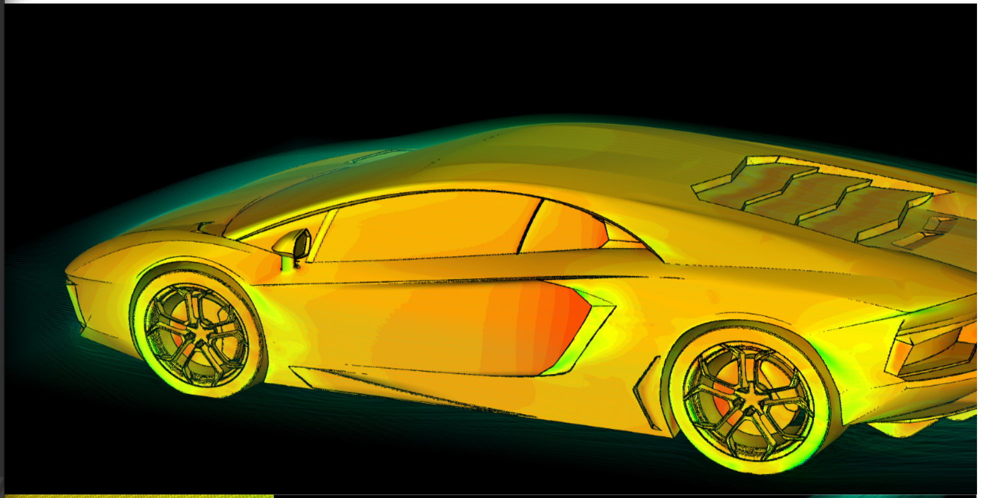
https://en.wikipedia.org/wiki/Navier–Stokes_existence_and_smoothness

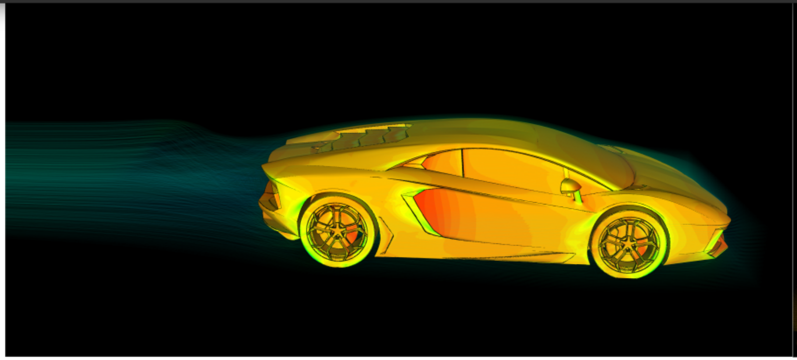
Parallel Computing

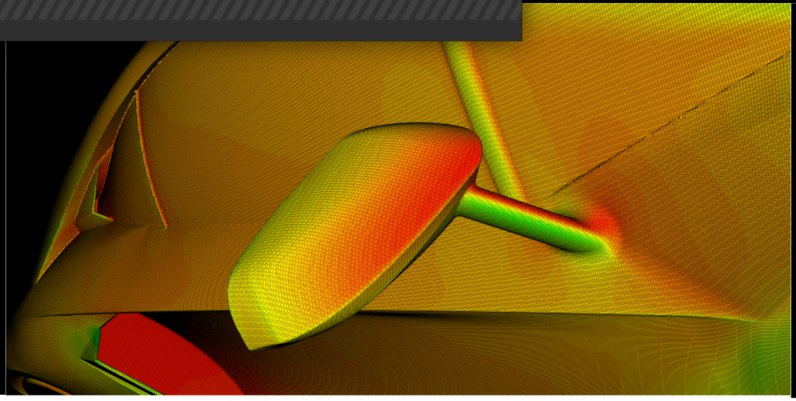
225.3 M Cells, 1351.8 M Unknowns
simpleFoam, k-omegaSST

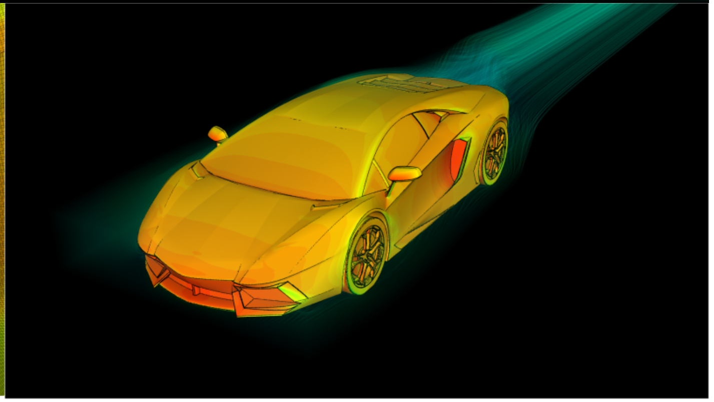
Mesh generated by snappyHexMesh in parallel
2000 time step iter.

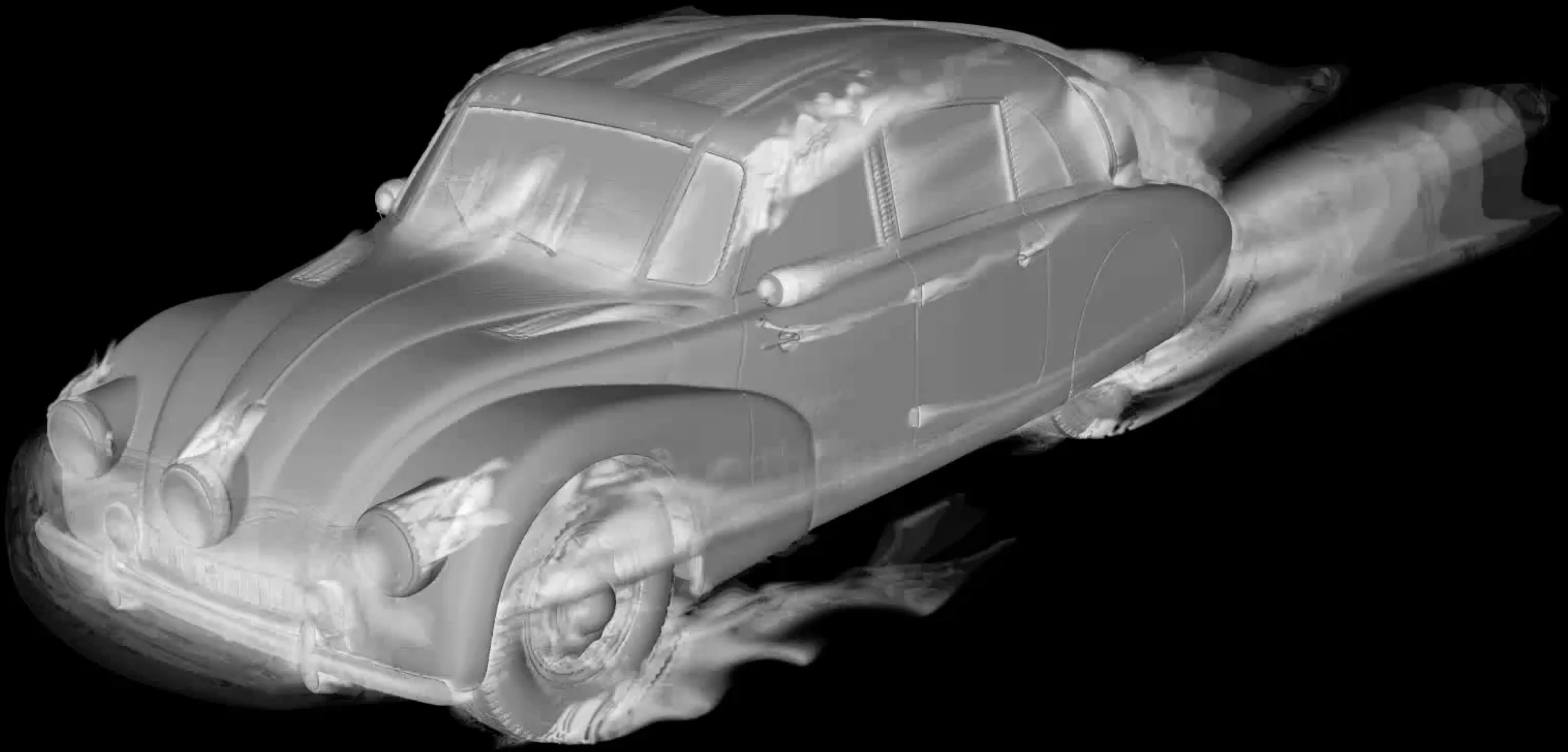




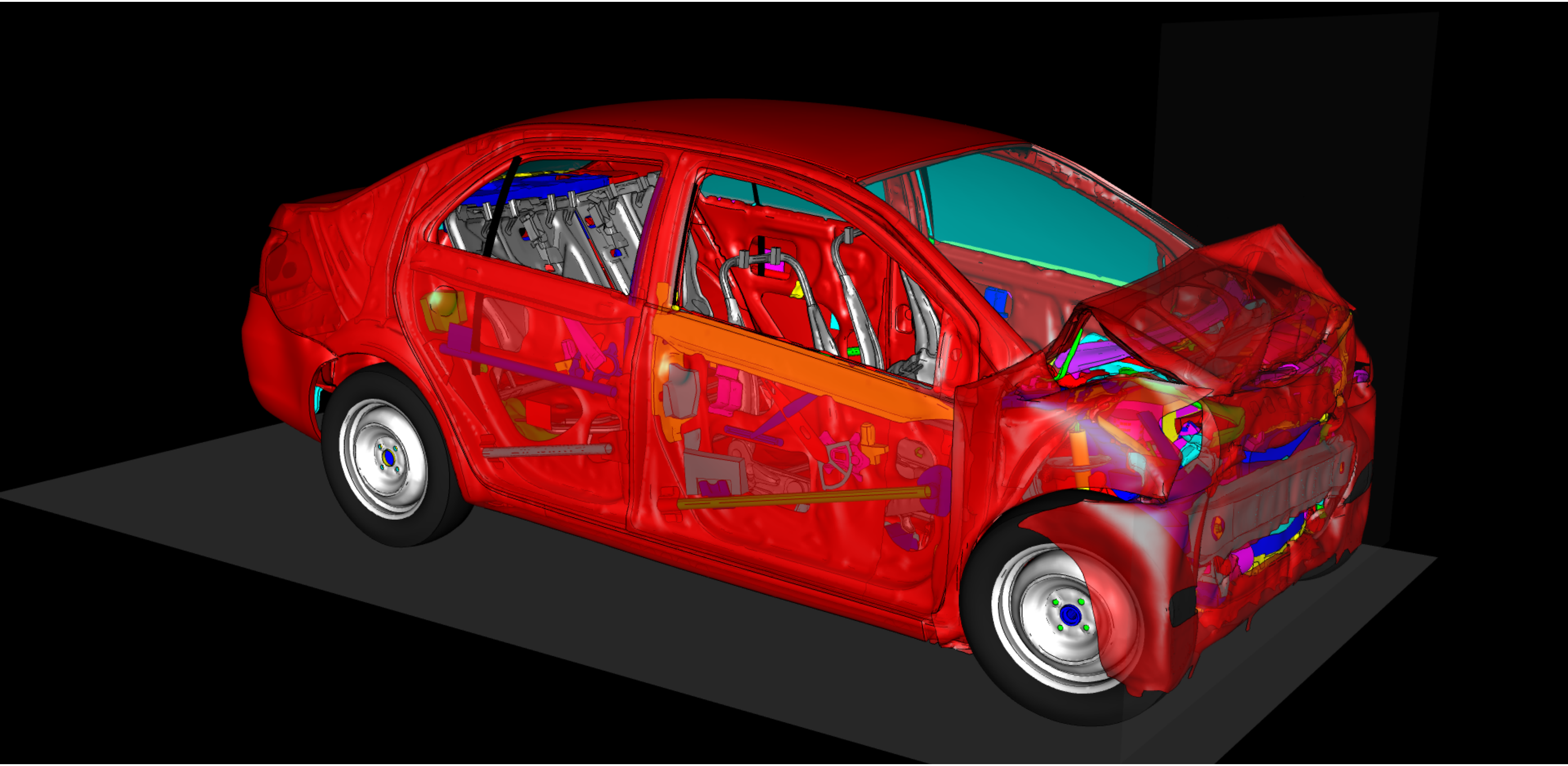


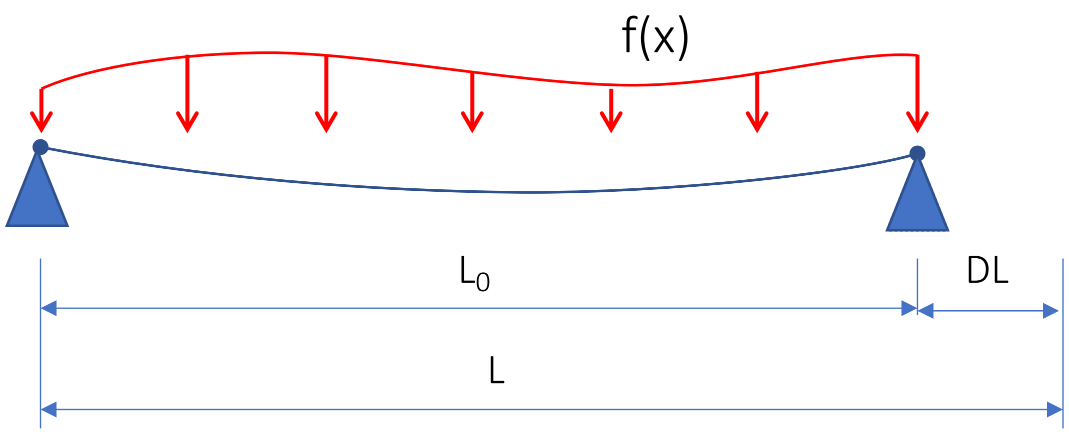


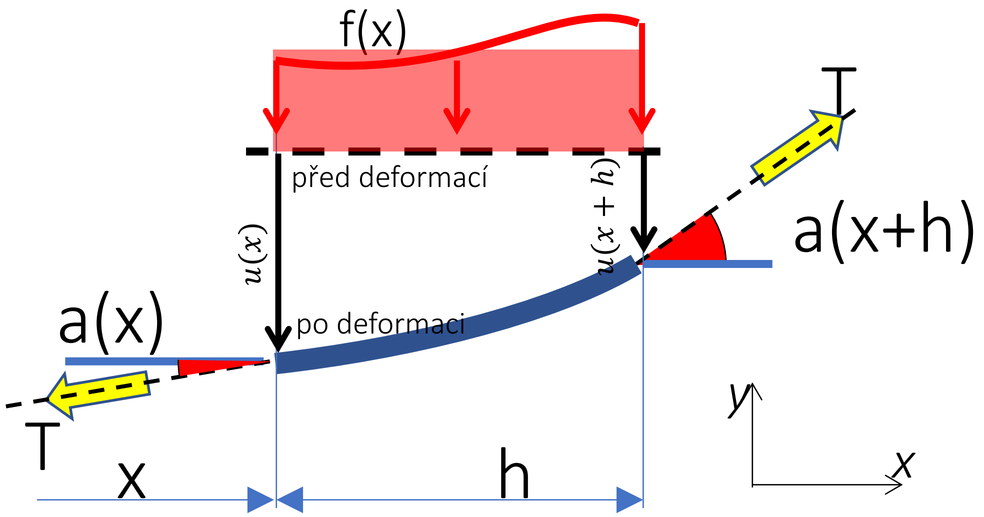




Structural mechanics







- Struna je **předepnuta** – natažena o délku DL

- Ve struně vznikne tzv. **předepínací síla T**, která je po celé délce konstantní

$$\sum F = 0 = -T\sin\alpha(x) + T\sin\alpha(x+h) + f\left(x + \tfrac{1}{2}h\right)h$$

$$-T\sin\alpha(x+h) + T\sin\alpha(x) = f\left(x + \tfrac{1}{2}h\right)h$$

$$-T\frac{\sin\alpha(x+h) - \sin\alpha(x)}{h} = f\left(x + \tfrac{1}{2}h\right)$$

$$\lim_{h\to 0} -T\frac{\sin\alpha(x+h) - \sin\alpha(x)}{h} = f\left(x + \tfrac{1}{2}h\right)$$

$$\sin\alpha(x) \approx \alpha(x) \approx \mathrm{tg}\alpha(x)$$

$$-T\left(\sin\alpha(x)\right)' = f(x)$$

$$\mathrm{tg}\alpha(x) = u'(x)$$

$$\boxed{-Tu''(x) = f(x)}$$

Známe:

- materiál, ze kterého je struna vyrobena
- zátěž v každém bodě struny (funkce ***f(x)***)
- uchycení (tvz. okrajové podmínky)

Hledáme:

- **deformaci** struny pod zatěžující liniovou silou

Rovnice rovnováhy v libovolném bodě struny

$$-Tu''(x) = f(x)$$

Eliptická parciální diferenciální rovnice druhého řádu

Poissonova rovnice:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f(x, y, z)$$

Laplaceova rovnice:

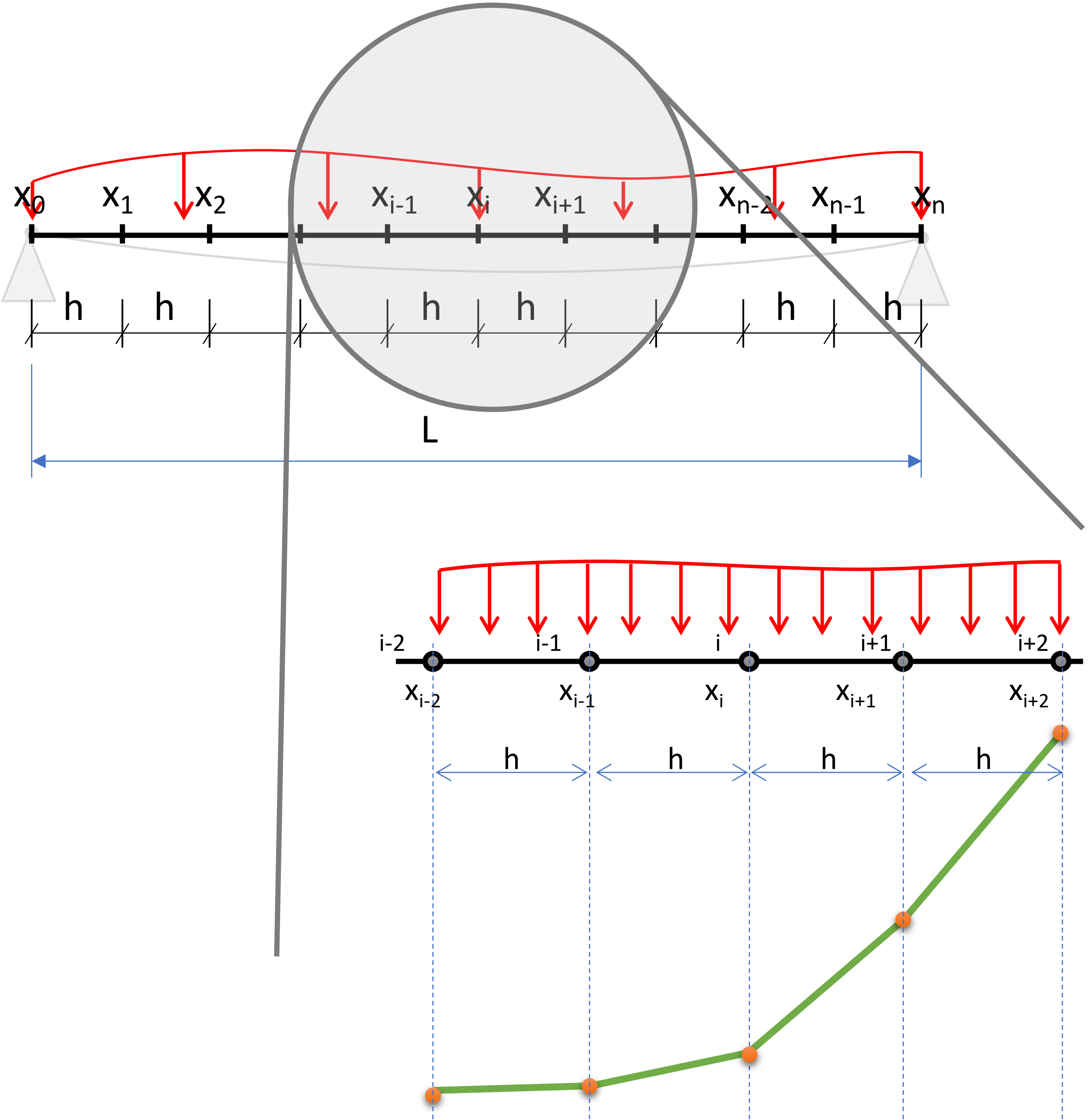
$$\Delta u = 0\,,$$

Analytické řešení - („přesné“)

- pro jednoduše matematicky popsatelné tvary
- Čtverec
- Kružnice
- Koule
- Válec
- nebo jejich kombinace v omezené míře

Numerické řešení - („přibližné“)

- Metoda sítí
- Metoda konečných objemů
- Metoda konečných prvků
- Metoda hraničních prvků
- Isogeometrická analýza
- …



Rovnice rovnováhy v libovolném bodě struny

$$-Tu''(x) = f(x)$$

Příklad soustavy po diskretizaci struny metodou sítí

$$\begin{pmatrix} 2 & -1 & 0 & & \cdots & 0 \\ -1 & 2 & -1 & 0 & & \vdots \\ 0 & -1 & 2 & -1 & \ddots & \\ & 0 & -1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & 2 & -1 \\ 0 & \cdots & & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{pmatrix} = \frac{h^2}{T} \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{pmatrix} + \begin{pmatrix} u_0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ u_n \end{pmatrix}$$

$$Ku = f$$

soustavu řešíme

- přímými řešiči (Gussova eliminace, ...)
- iteračními řešiči (sdružené gradienty, ...)

Second order elliptic partial differential equation

Laplace equation:

$$\Delta u = 0,$$

Poisson equation :

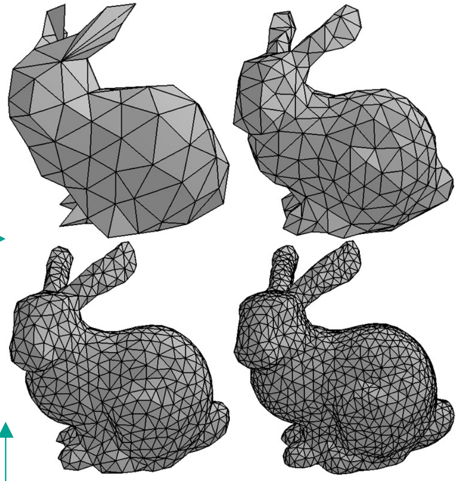
$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f(x, y, z)$$

Advection diffusion reaction equation

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\vec{v} c) + R$$

Numerical methods

Space discretization



optimization loop
    time loop
        nonlinear loop
            linear system solution – HPC
        end
    end
end

$$Ku = f?$$

Heat transfer

Software

- Creating complex model, computational mesh, boundary condition definition, material models – preProcesing
- Solution by numerical methods
- Results analysis- postProcessing

Open source: OpenFOAM, Code Saturne, SU^2, Elmer,…
https://www.cfd-online.com/Wiki/Codes#Free_codes

Commercial codes: ANSYS CFD, FLUENT, CFX, StarCCM+,…
https://www.cfd-online.com/Wiki/Codes#Commercial_codes

Or try to write it in your own way
Matlab,R, Octave, Python, C, C++, Fortran…

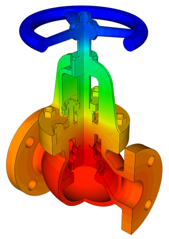
ESPRESO FEM Highly parallel finite element package for engineering simulations

Heat Transfer Module Capability List:

Load steps definition for combination of multiple steady-state and time dependent analyses

Transient solvers

- Generalized trapezoidal rule
- Automatic time stepping based on response frequency approach

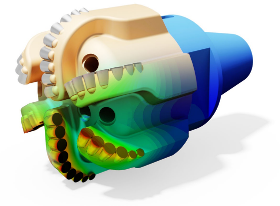


Nonlinear solvers

- Newton Raphson – full and symmetric
- Newton Raphson with constant tangent matrices
- Line search damping
- Sub-steps definition
- Adaptive precision control for iterative solvers

Linear and quadratic finite element discretization

Gluing nonmatching grids by mortar discretization techniques



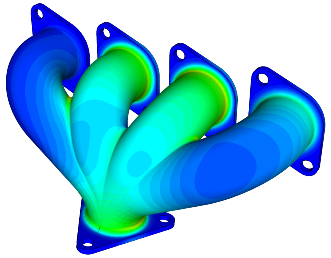
Full-fledged material models

- nonlinear materials
- isotropic, orthotropic and anisotropic material models
- materials for phase change

Element coordinate system definition – cartesian, polar and spherical

Temperature and time dependent boundary conditions

- linear convection
- nonlinear convection
- heat flow
- heat flux
- diffuse radiation
- heat source
- translation motion



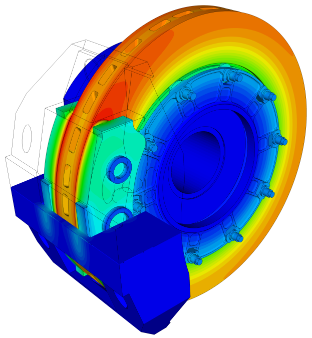
Consistent SUPG and CAU stabilization for Translation Motion (advection), Inconsistent stabilization

Phase Change based on apparent heat capacity method

Boundary element discretization for selected physical applications

Highly parallel multilevel FETI domain decomposition based solver for billions of unknowns for symmetric and non-symmetric systems with accelerators support and combination of MPI and OpenMP techniques

Asynchronous parallel I/O

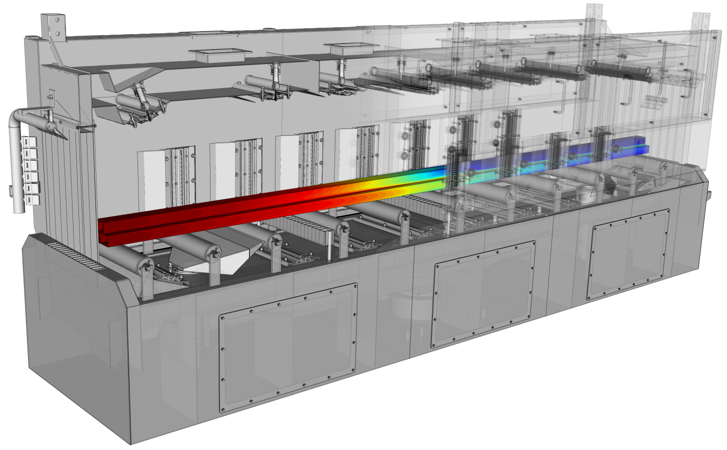


Input mesh format from popular open source and commercial packages like OpenFOAM, ELMER or ANSYS

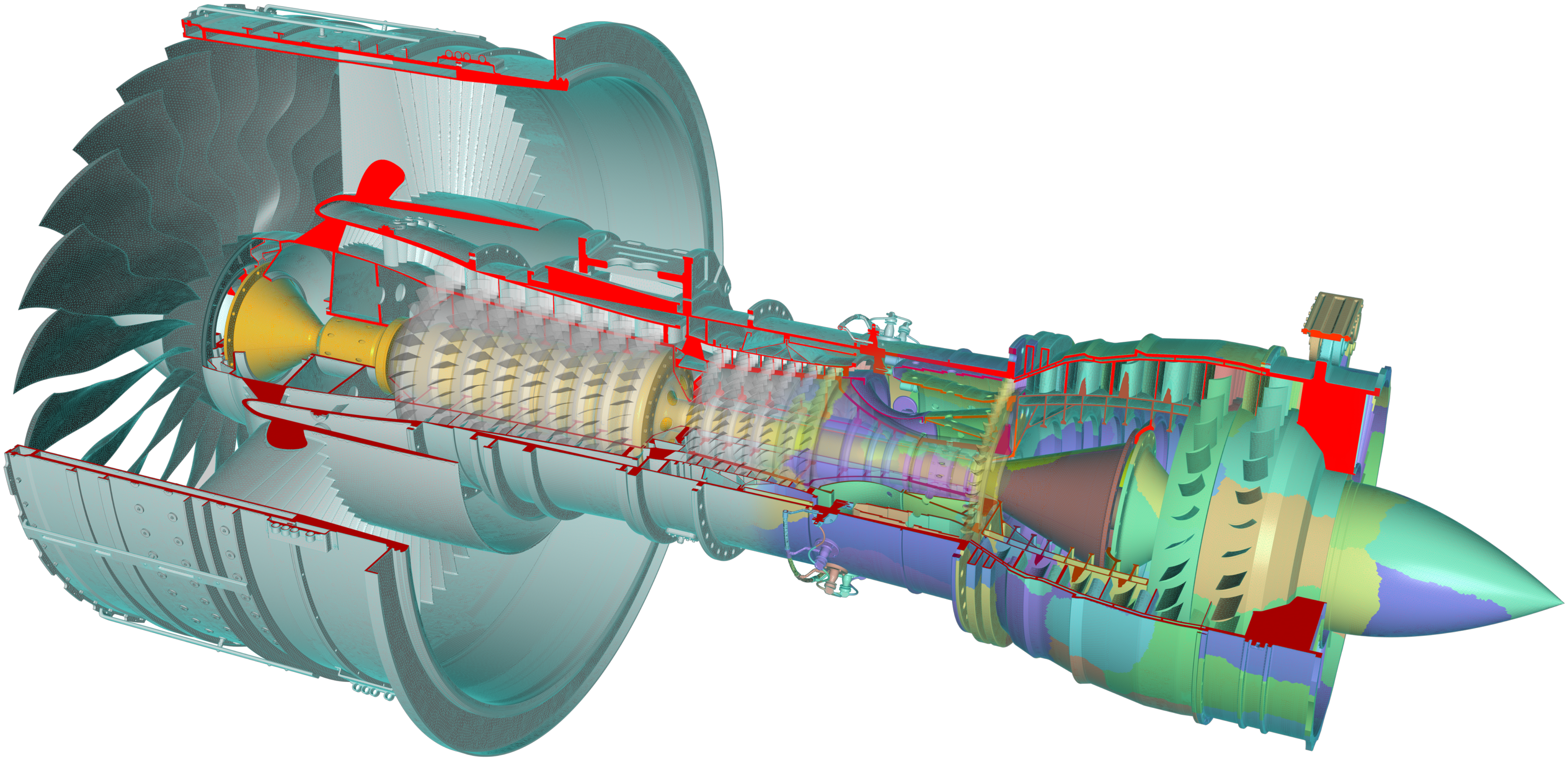
Output to commonly used post-processing formats, VTK and EnSight

Monitoring results on selected regions for statistic and optimization toolchain

Simple text Espreso Configuration File (ecf) for setting all ESPRESO FEM solver parameters without GUI. Control each parameter in ecf file from command line

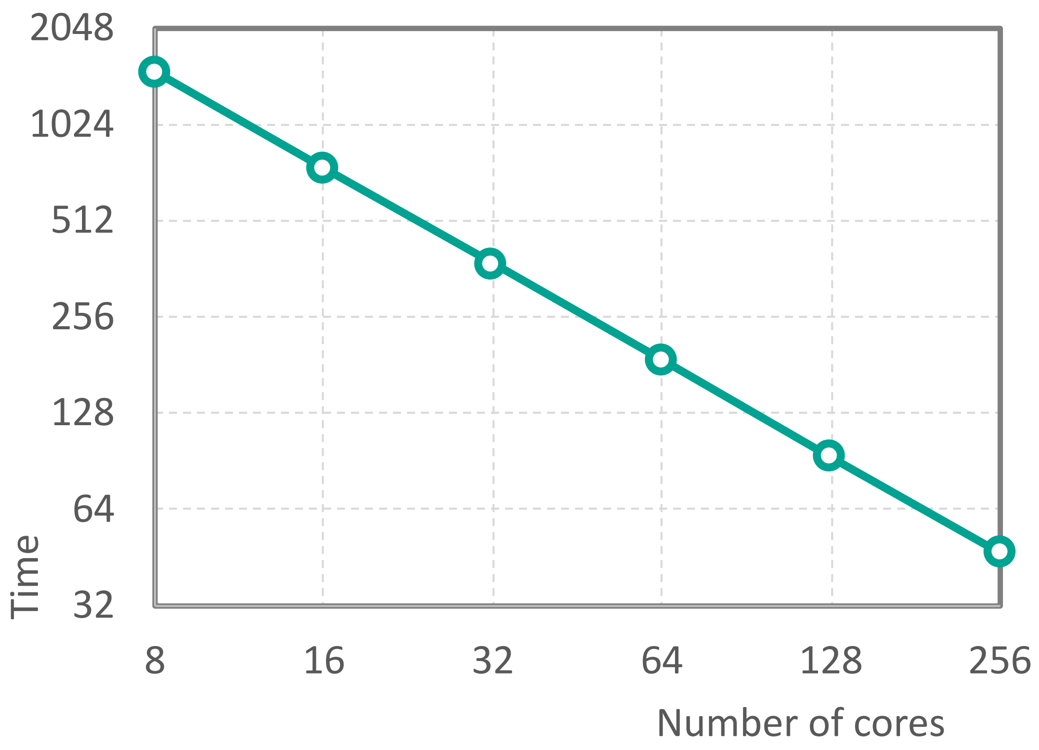


ESPRESO FEM Highly parallel finite element package for engineering simulations

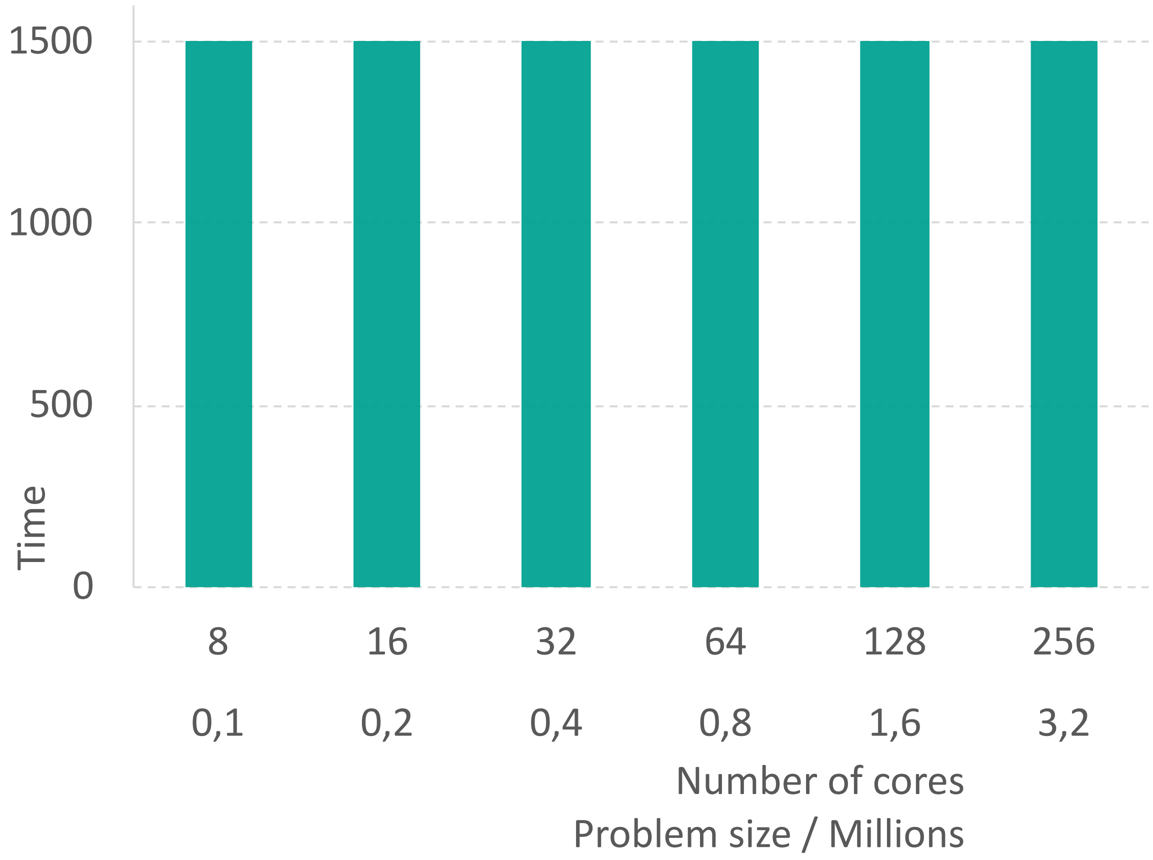


Behaviour of numerically and parallel scalable solvers

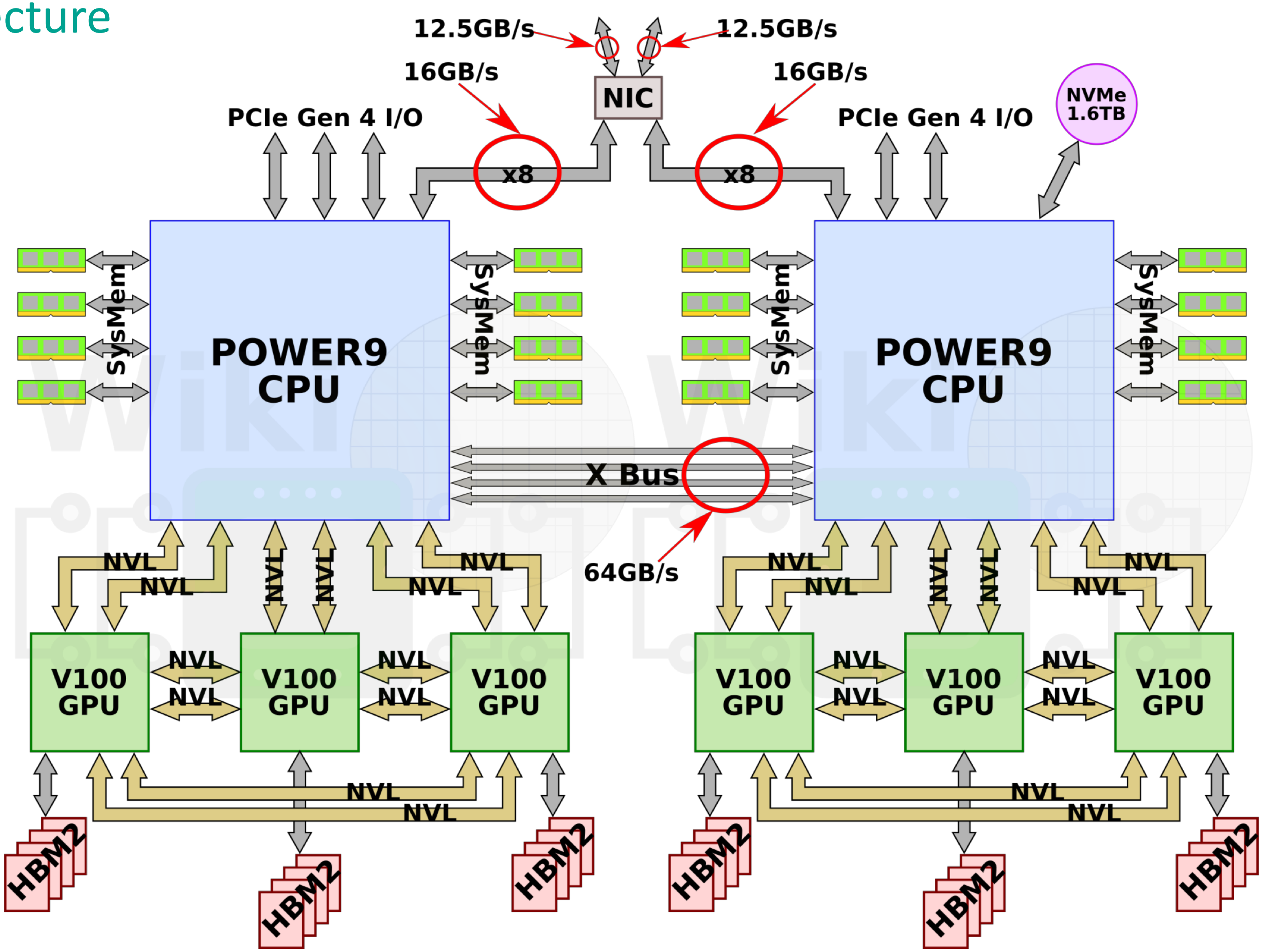
Parallel (strong) Scalability



Numerical (weak) Scalability



Hybrid architecture



ESPRESO on TITAN

3rd (9th) in TOP500 LIST

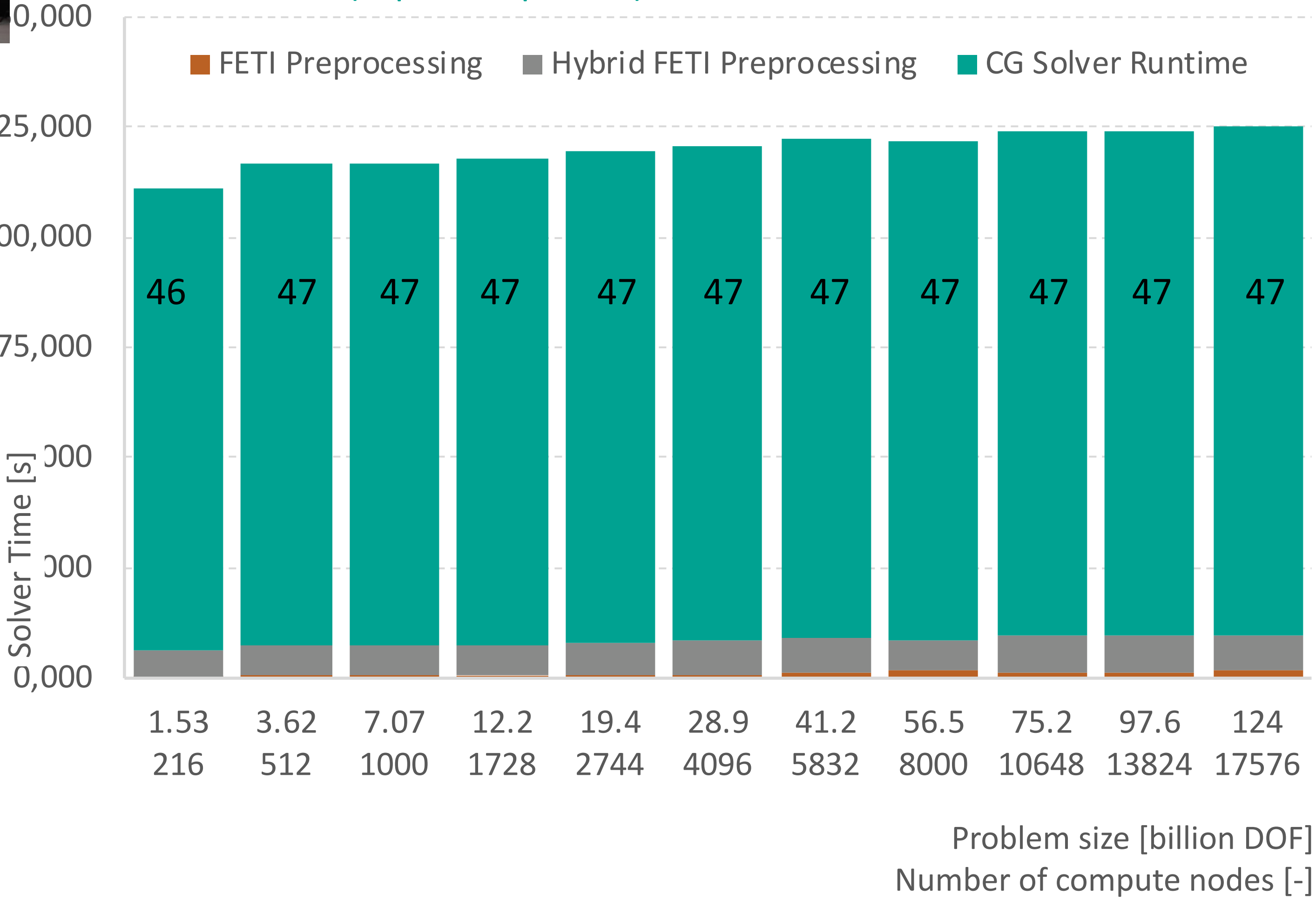
18,688   AMD Opteron 6274 16-core CPUs
18,688   Nvidia Tesla K20X GPUs

2.7 million core hours dedicated to:
- scalability optimization of ESPRESO
- optimization of GPU accelerated version for large scale problems

OAK RIDGE National Laboratory

Weak Scalability Test

Up to **124 billion** DOF on 17576 Compute Nodes (281 216 cores)
Heat transfer (Laplace equation)

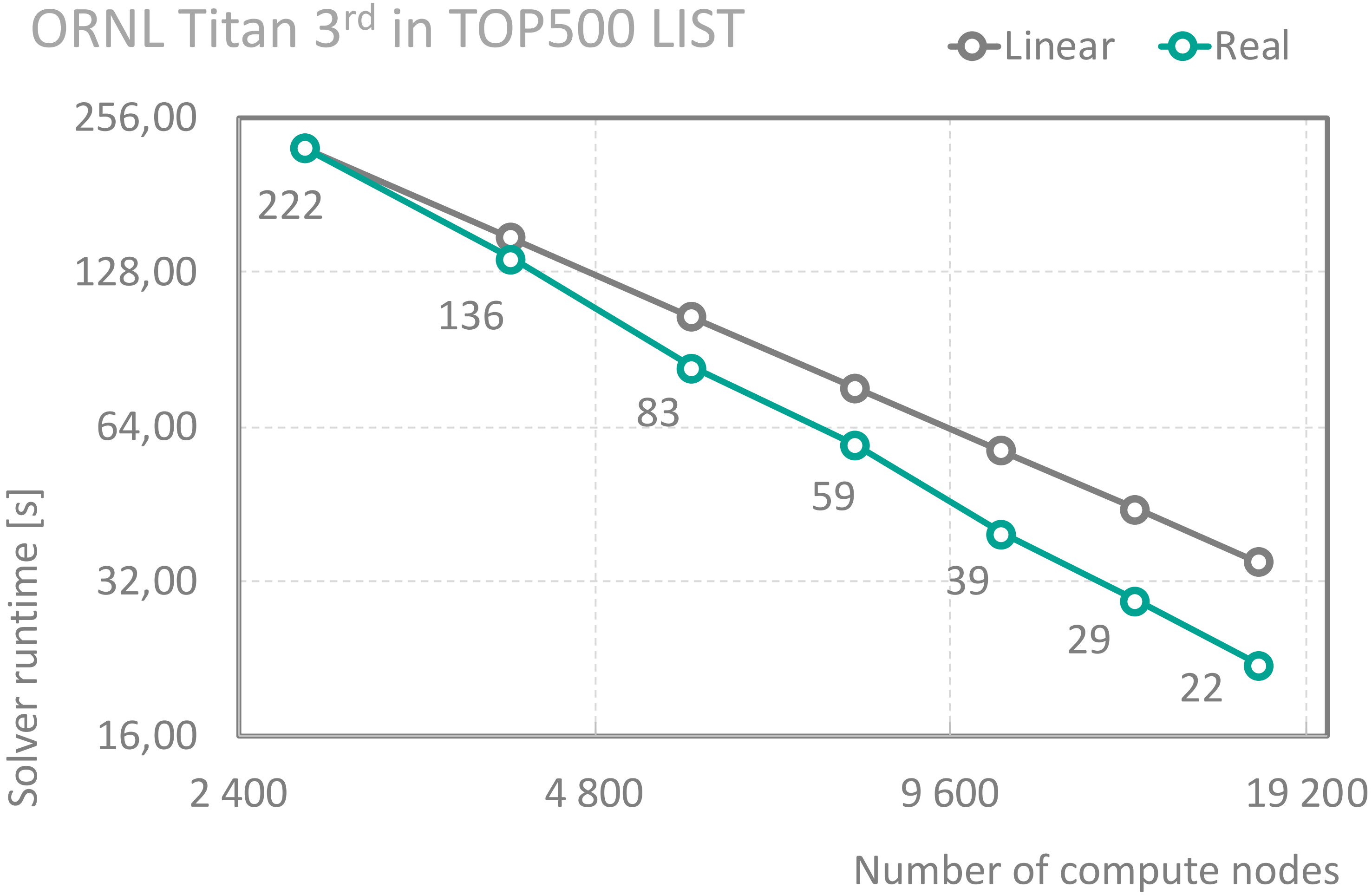


Strong Scalability Test

20 billion DOF on up to 17 576 Compute Nodes (281 216 cores)

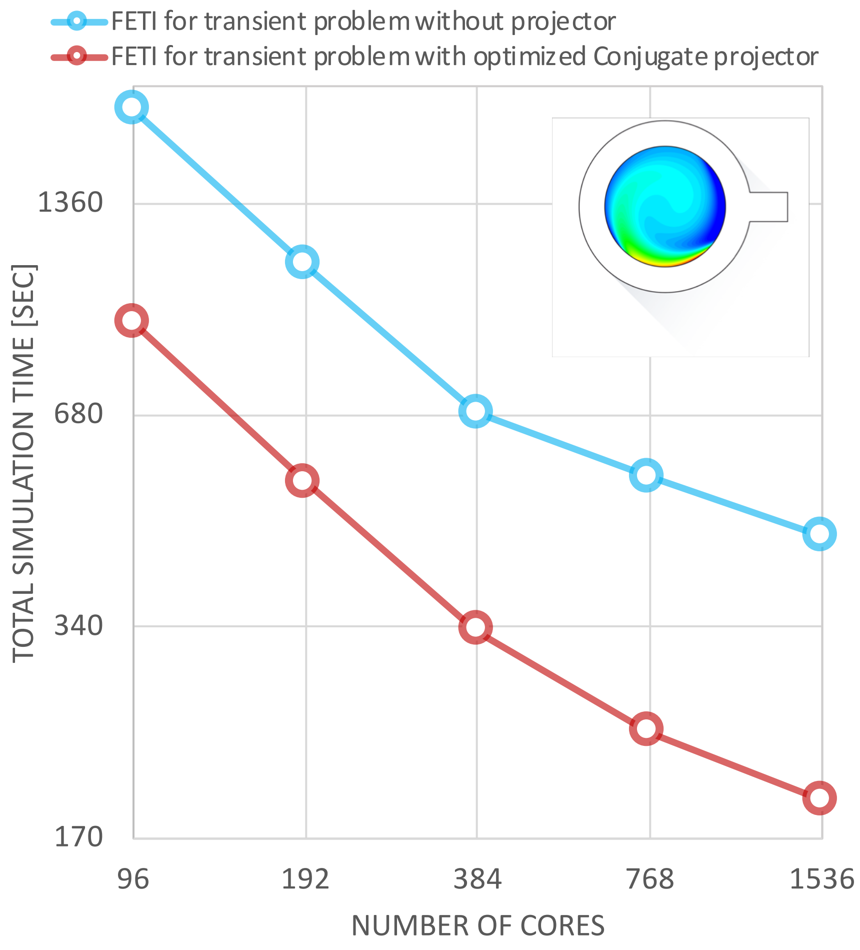
Heat transfer (Laplace equation)

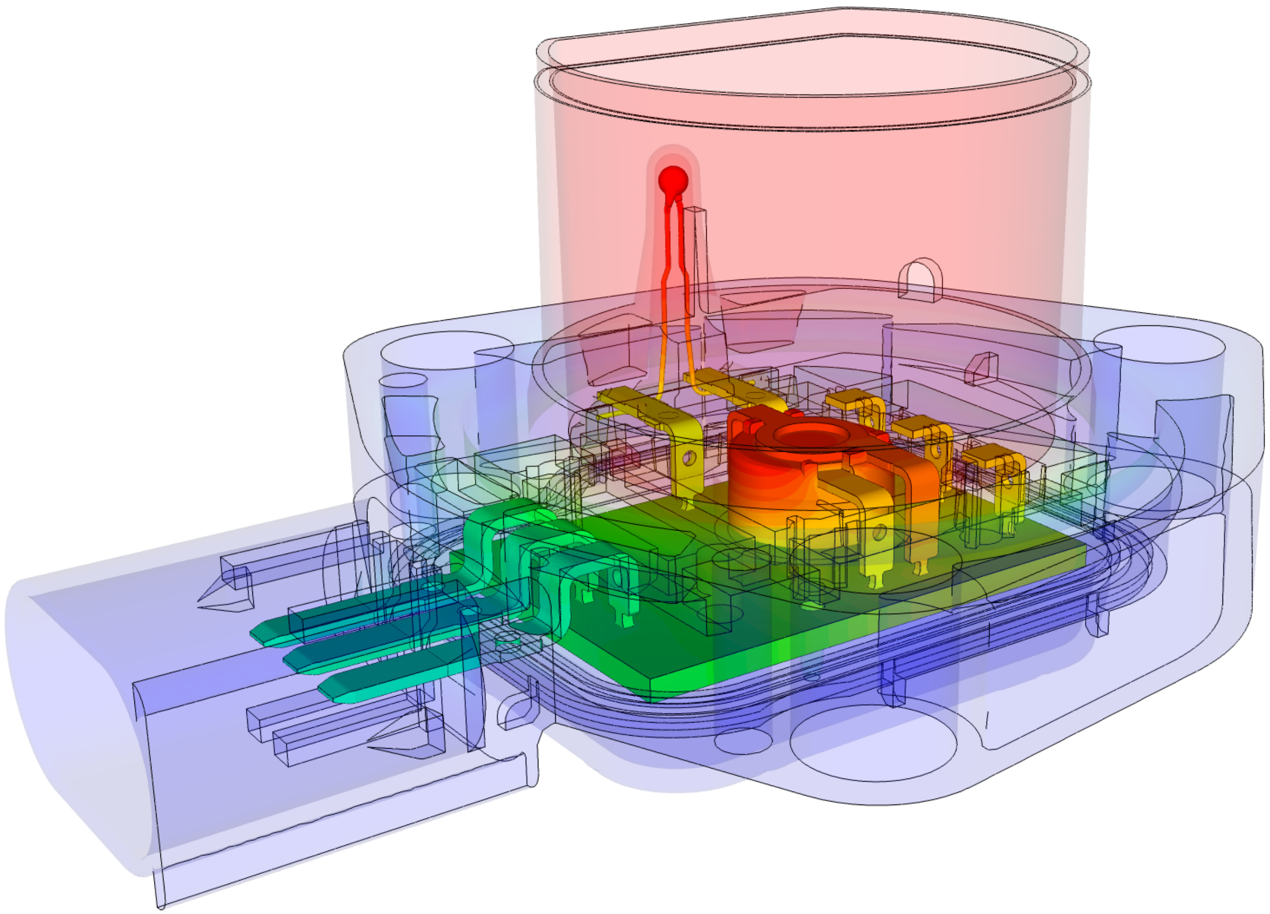
ORNL Titan 3rd in TOP500 LIST



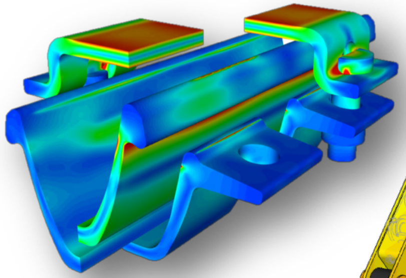
Latent heat distribution in the wheel

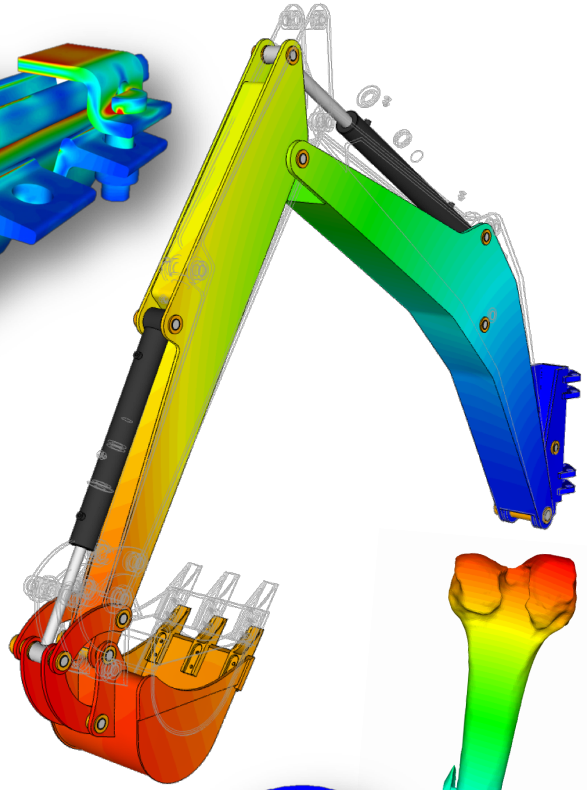
Response time optimization of the USL sensor - nonlinear transient simulation





Structural mechanics





Elasticity BVP

$$
\begin{aligned}
-\mathrm{div}\boldsymbol{\sigma}^{(k)} &= \mathbf{f}^{(k)} && \text{in } \Omega^{(k)}\\
\sigma_{ij}^{(k)} &= c_{ijkl}\varepsilon_{kl}^{(k)} && \text{in } \Omega^{(k)}\\
\varepsilon^{(k)} &= \frac{1}{2}\left(\nabla\mathbf{u} + \nabla^\top\mathbf{u}\right) && \text{in } \Omega^{(k)}\\
\mathbf{u}^{(k)} &= \mathbf{0} && \text{on } \Gamma_D^{(k)}\\
\boldsymbol{\sigma}^{(k)}\mathbf{n}^{(k)} &= \mathbf{t}^{(k)} && \text{on } \Gamma_N^{(k)}
\end{aligned}
$$

Terms on contact boundary

$$
\begin{aligned}
-g(\mathbf{X}) &= u_n(\mathbf{X}) - d(\mathbf{X})\\
\mathbf{t}_C^m \,\mathrm{d}\gamma_C^m &= -\mathbf{t}_C^s \,\mathrm{d}\gamma_C^s\\
\mathbf{t}_C^s &= t_n\mathbf{n} + t_{1T}\boldsymbol{\tau}_1 + t_{2T}\boldsymbol{\tau}_2
\end{aligned}
$$

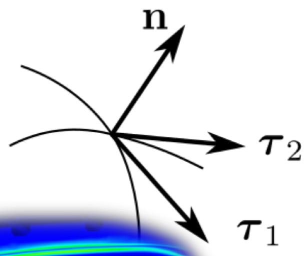
Unilateral contact (non-penetration)

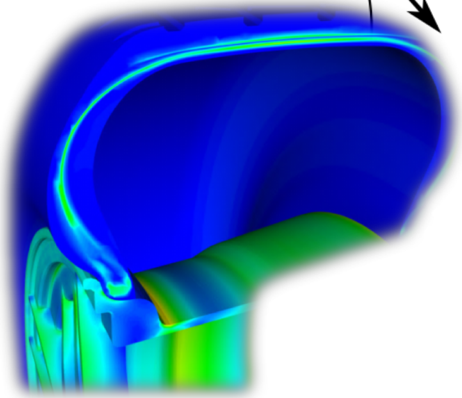
$$
u_n - d \le 0,\ t_n \le 0,\ t_n(u_n - d) = 0
$$

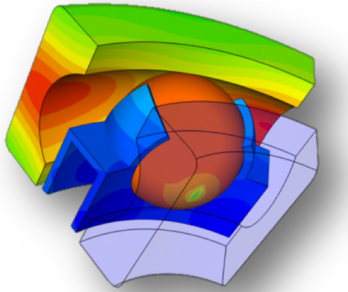
Friction (Tresca or Coulomb)

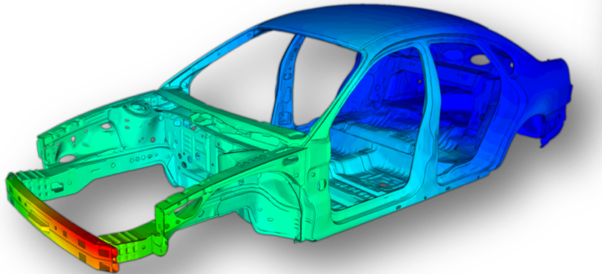
$$
\|\mathbf{t}_T\|_2 \le F,\ \begin{cases} \|\mathbf{t}_T\|_2 < F & \Rightarrow\ \mathbf{u}_T = \mathbf{0}\\ \|\mathbf{t}_T\|_2 = F & \Rightarrow\ \mathbf{u}_T = -c\mathbf{t}_T,\ c \ge 0 \end{cases}
$$

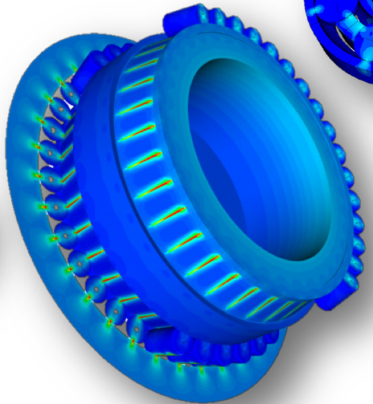
$$
F = \begin{cases} sb & \ldots\ \text{Tresca}\\ \mathscr{F}|t_n| & \ldots\ \text{Coulomb} \end{cases}
$$

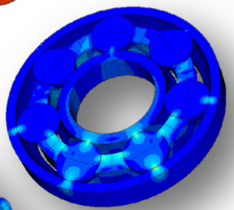


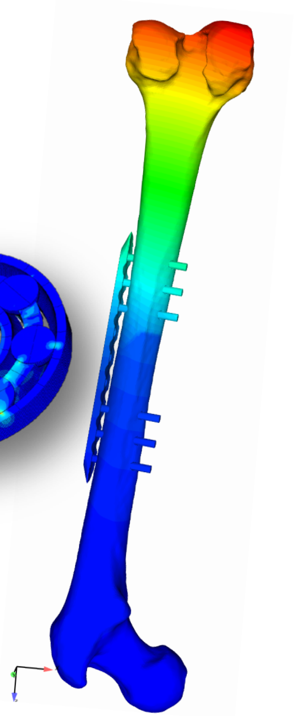












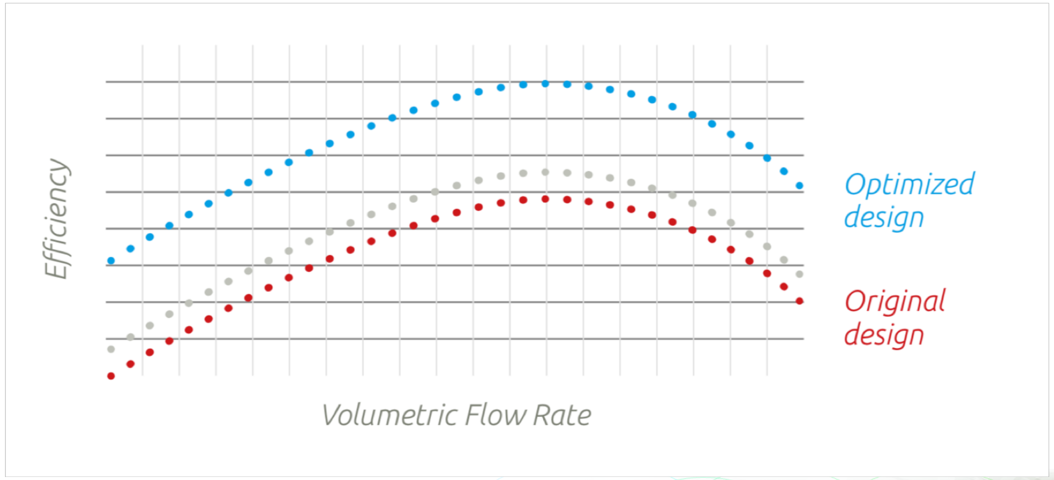
Digital Twin Technology

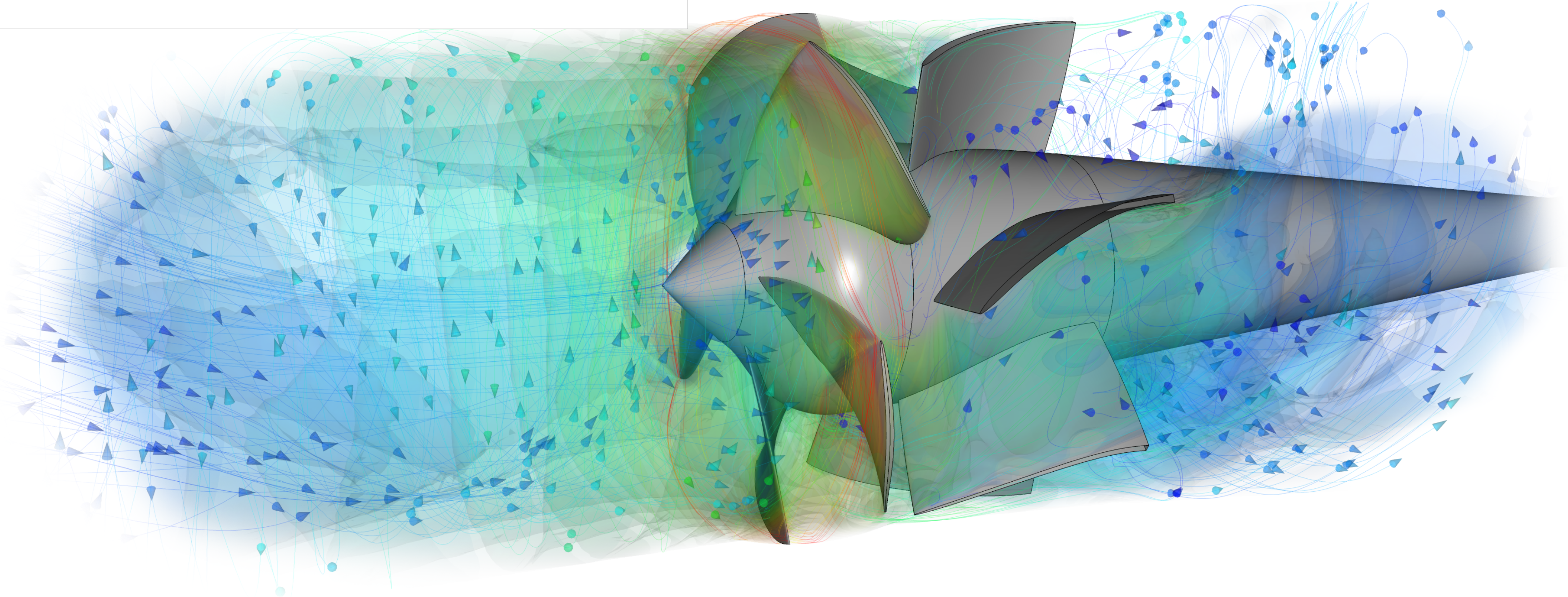
Multiphysics simulations

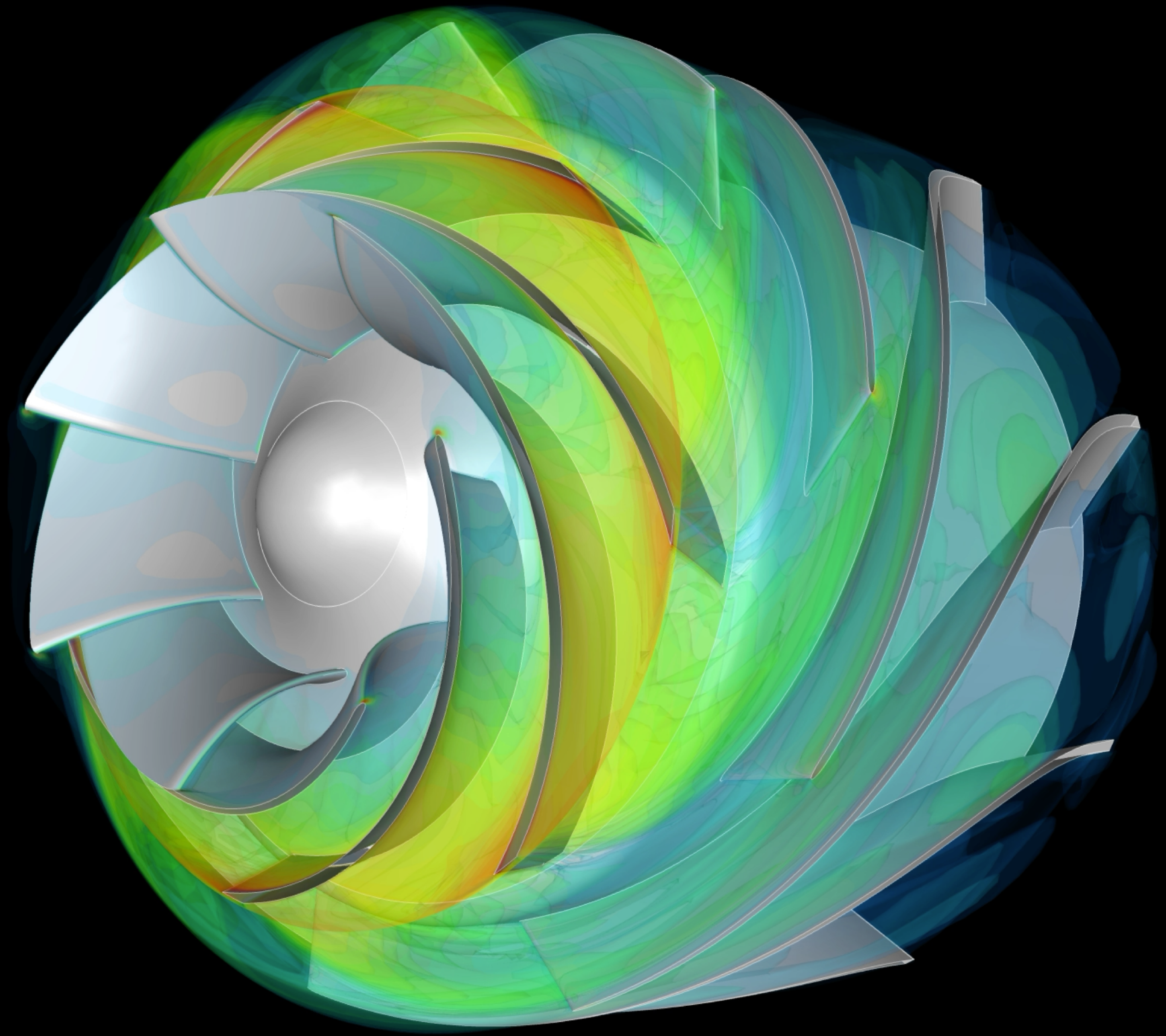
Complex nonlinear multiphysical problem – electric motor

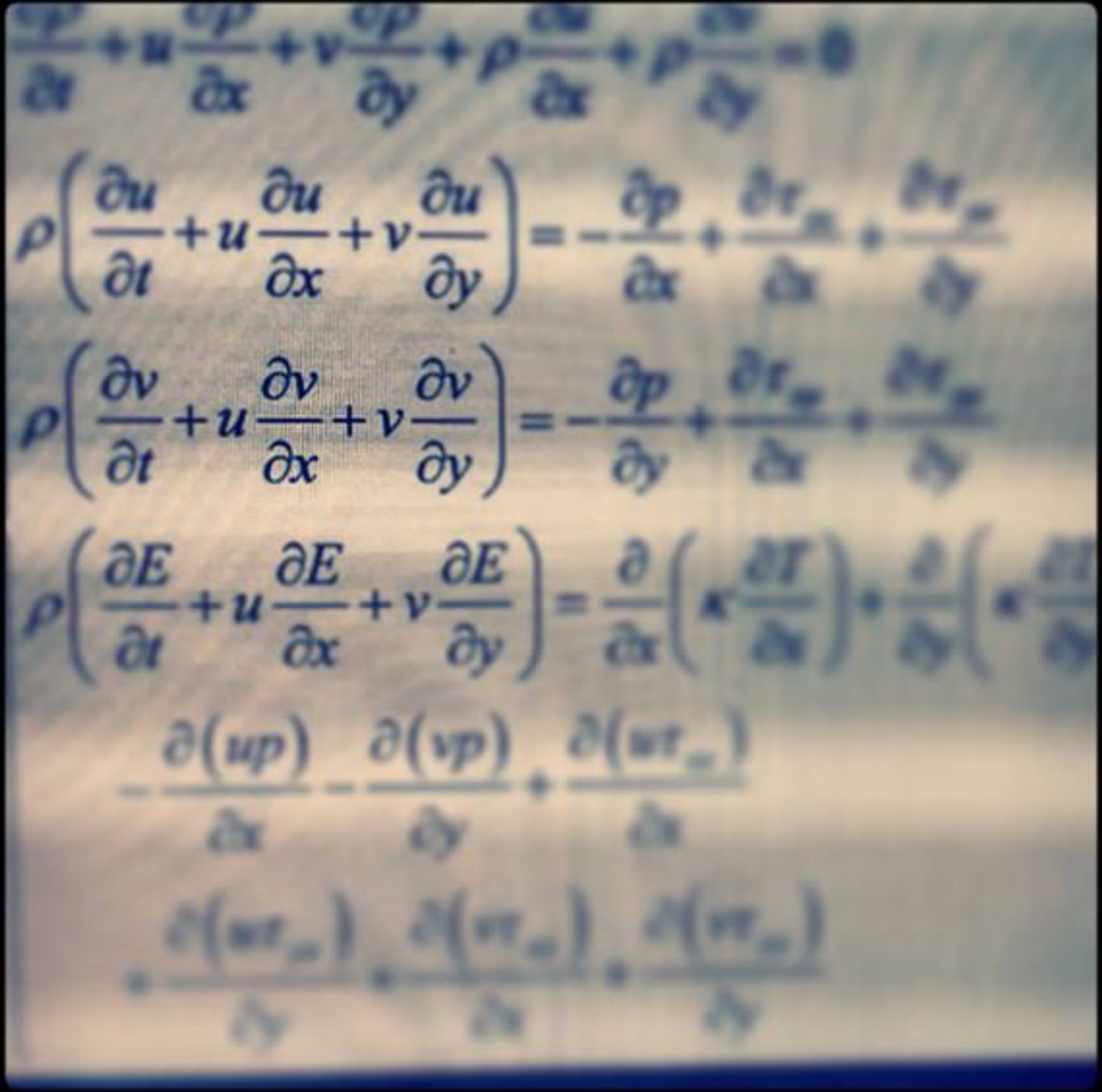
- Electric fields
- Electromagnetism
- Heat transfer
  - heat generated by magnetism
  - cooling system
- Structural Mechanics
  - structural integrity
  - vibration from motion
  - high speed motors
  - influenced by electromagnetism
- Active cooling system
  - fluid flow
- Acoustic
  - generated by fluid flow
  - generated by electromagnetism
  - generated by vibrations

Water pump efficiency optimization









Parallel algorithms research lab
IT4Innovations National Supercomputing Center
VSB - Technical University of Ostrava
Studentská 6231/1B
708 33 Ostrava-Poruba
Czech Republic
www.it4i.cz

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER