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Applications of Large-Scale Nonlinear Optimization at the Petascale: Achievements and perspectives

February 4, 2014

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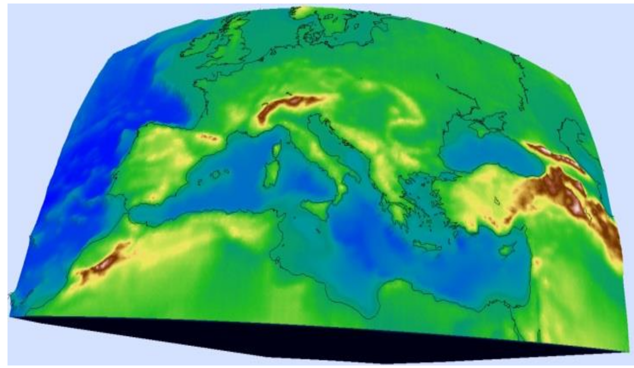
Institute of Computational Science
Universita della Svizzera italiana, Lugano

Applications of Large-Scale Optimization and HPC

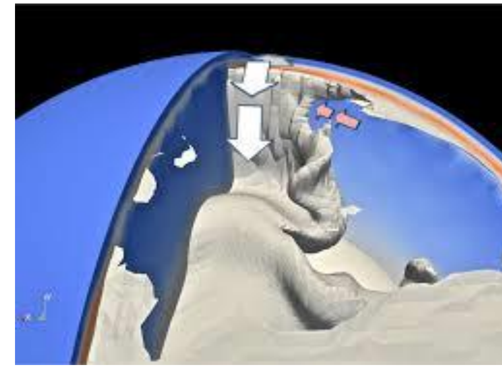
Power-Grid Optimization under Uncertainty (Stochastic Programming)

DOE INCITE Project (Argonne, USI)



Computational Wave Propagation

SNF Projects (2006-…)



Seismic Inversion / Global Tomography

EU projects /HP2C (2010- …)

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

$$
\begin{aligned}
&\min_{\mathbf{x}} \; F(\mathbf{x}) \\
&\text{subject to} \quad c_i(\mathbf{x}) = 0 \qquad \text{for } i \in \mathcal{E} \\
&\qquad\qquad\quad\;\; c_i(\mathbf{x}) \geq 0 \qquad \text{for } i \in \mathcal{I}
\end{aligned}
$$

PASC Platform for Advanced Scientific Computing

HP2C High Performance and High Productivity Computing

Cray XC30 „Piz Daint", Switzerland, 2014

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ \textbf{s.t.} \quad & c(x) = 0 \\ & x \geq 0 \end{aligned}$$

- **User Lab for Swiss Scientists**
- **115'984 cores - 272 TB of RAM**
- **4PB TB local disks**
- **Size**
  - 23 t
  - 47 m^2
  - 2,325 MW

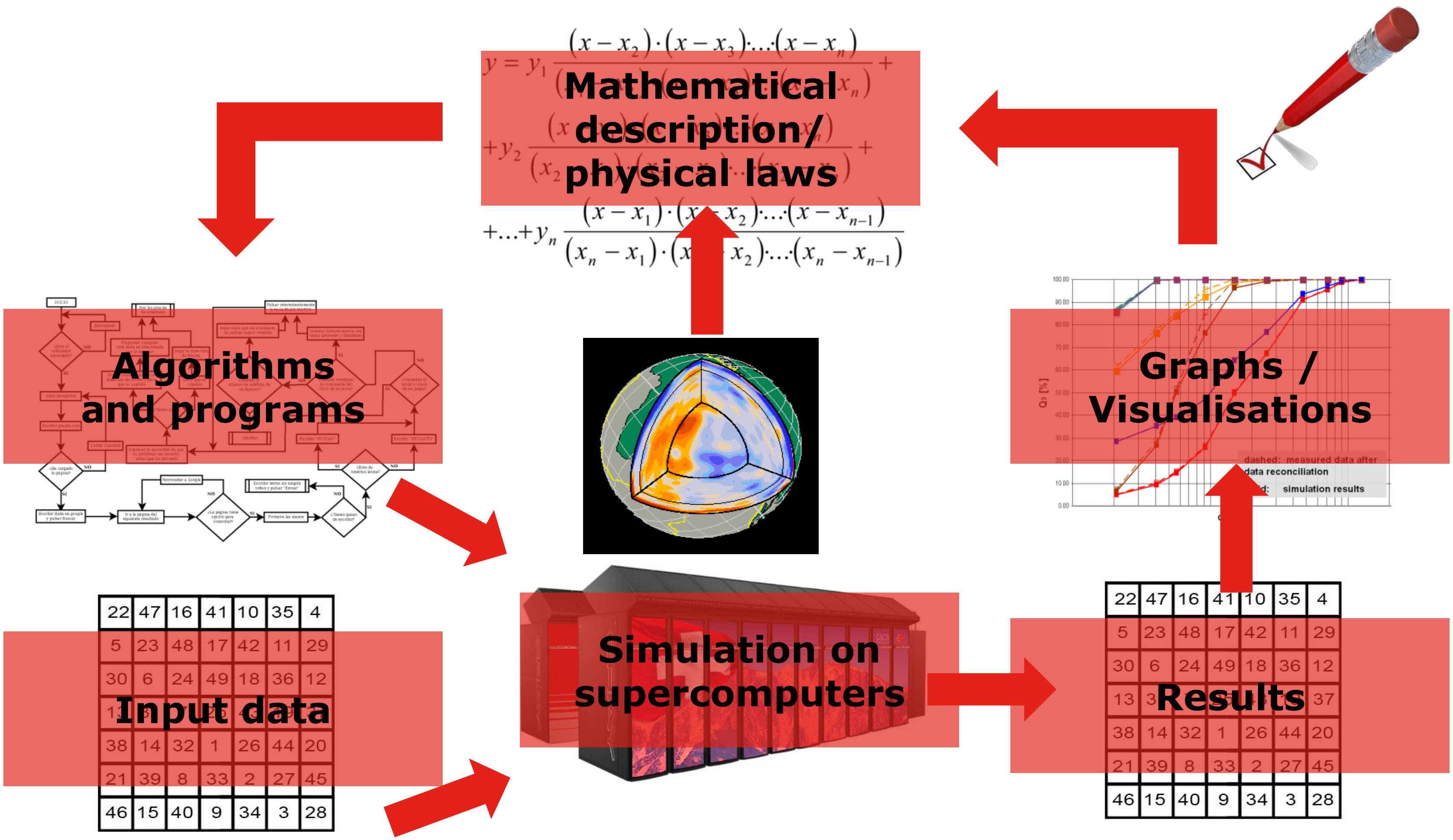
6,700 PFlops

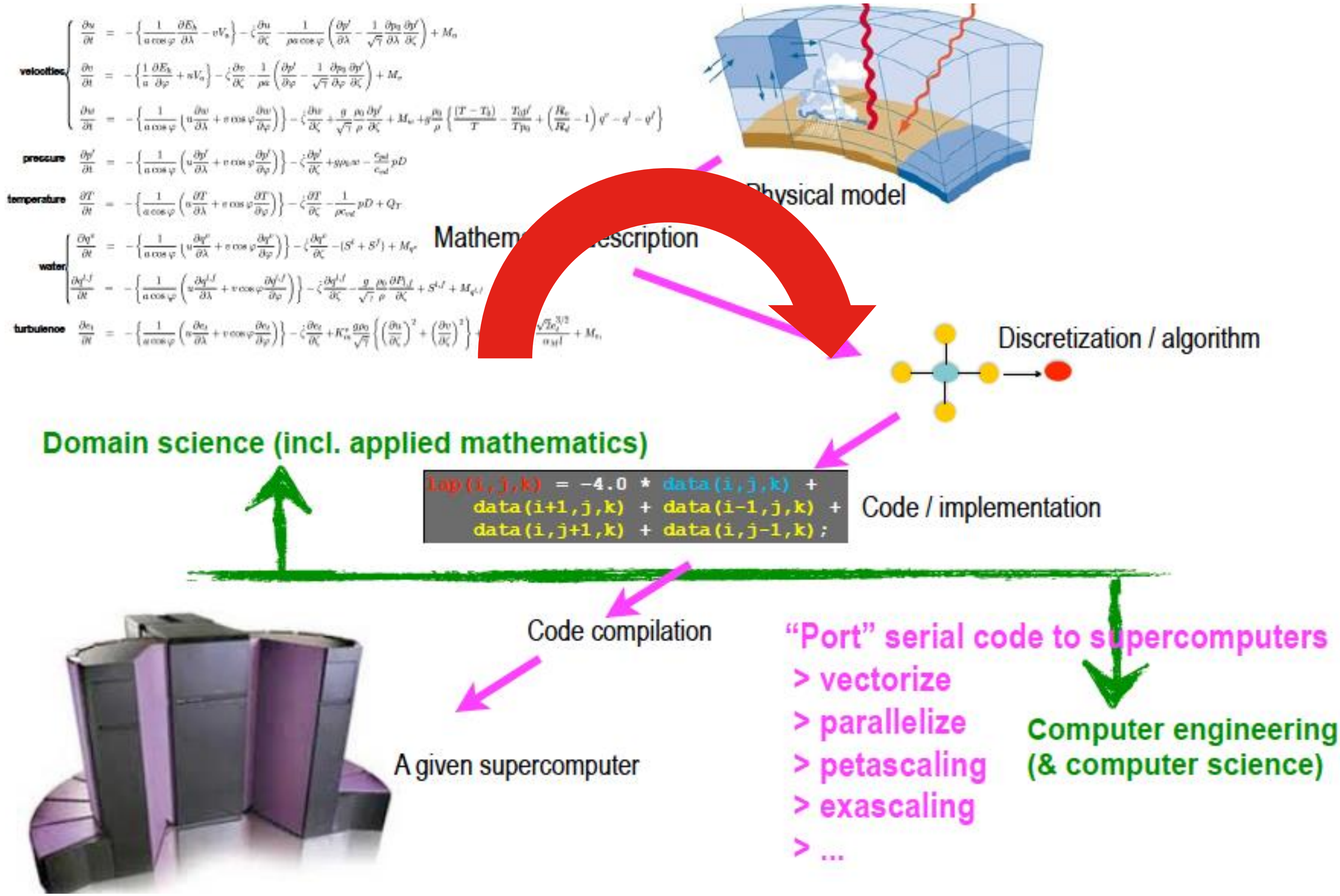
Agenda

- **Short portrait of**
  - HP2C and PASC, Swiss National Supercomputing Centre CSCS
- **Why supercomputing?**
  - Supercomputing and Computational Science
- **The challenge**
  - Co-Design of applications, software, and (hardware)
- **Interior-point methods for large scale stochastic optimization on high-performance computers**
  - Complementarity conditions
  - Linear algebra: LP, QP and NLP
  - Very Large-Scale Optimization
  - Stochastic, semi-structured optimization
  - Seismic Inversion & Power grid optimization under uncertainty

Why supercomputing?

How do computational scientists work?




velocities
pressure
temperature
water
turbulence
hysical model
Mathem
escription
Discretization / algorithm
Domain science (incl. applied mathematics)
lap(i,j,k) = -4.0 * data(i,j,k) +
data(i+1,j,k) + data(i-1,j,k) +
data(i,j+1,k) + data(i,j-1,k);
Code / implementation
Code compilation
A given supercomputer
“Port” serial code to supercomputers
> vectorize
> parallelize
> petascaling
> exascaling
> ...
Computer engineering
(& computer science)

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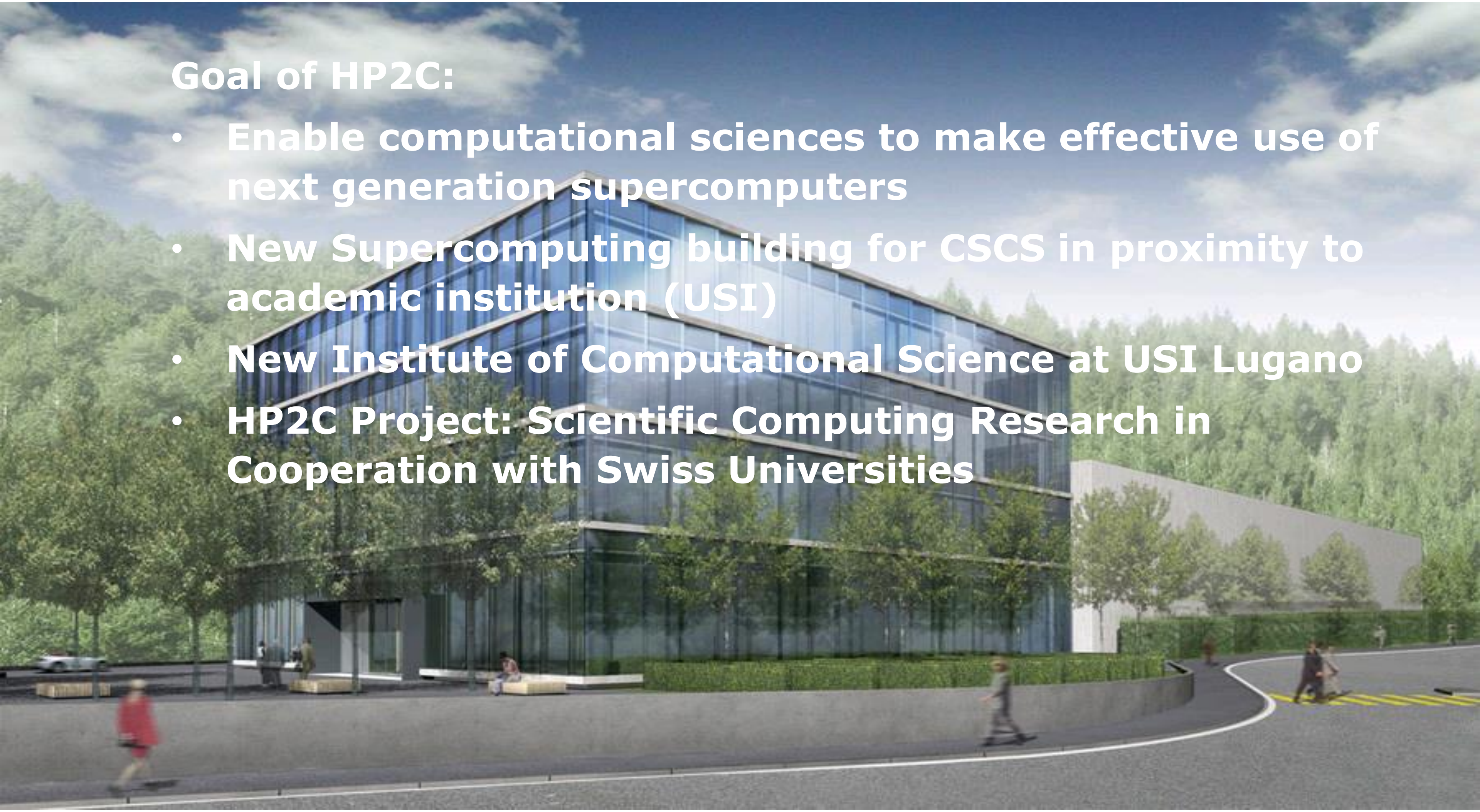
The Swiss platform for High-Performance and High-Productivity Computing (2010-2013)



Goal of HP2C:

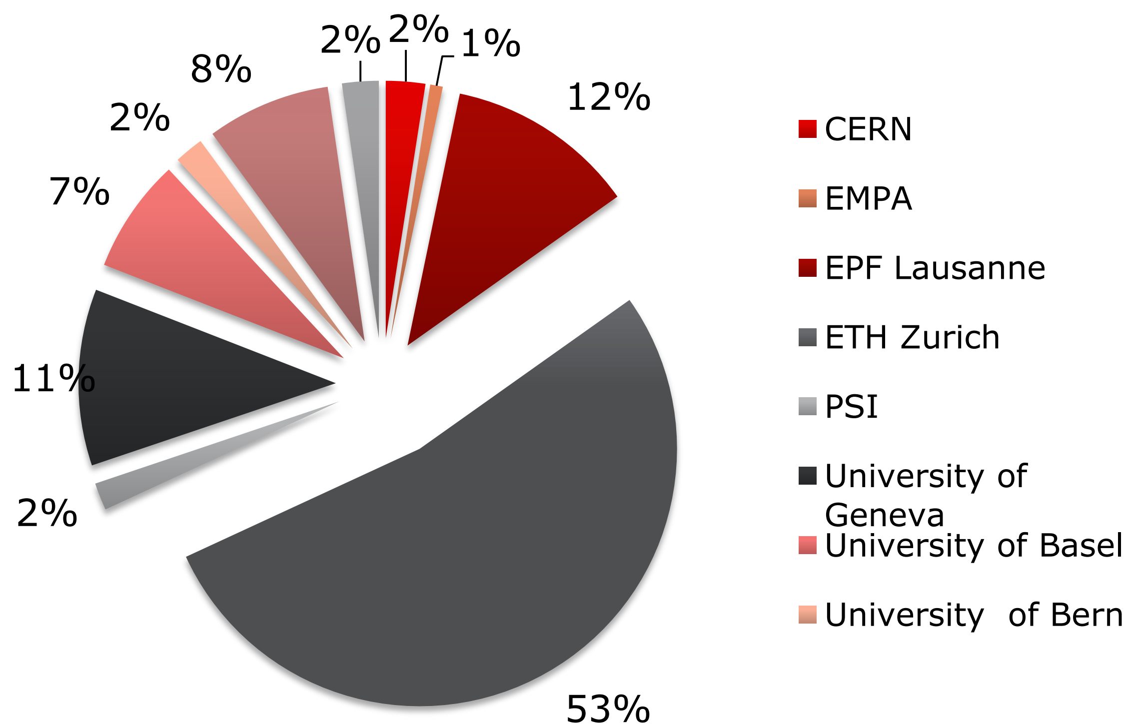
- **Enable computational sciences to make effective use of next generation supercomputers**
- **New Supercomputing building for CSCS in proximity to academic institution (USI)**
- **New Institute of Computational Science at USI Lugano**
- **HP2C Project: Scientific Computing Research in Cooperation with Swiss Universities**

CSCS in a nutshell

- **An autonomous unit of the Swiss Federal Institute of Technology in Zurich (ETH Zurich)**
  - founded in 1991 in Manno
  - relocated to Lugano in 2012
- **Develops and promotes technical and scientific services**
  - for the Swiss research community in the field of high-performance computing
- **Enables world-class scientific research**
  - by pioneering, operating and supporting leading-edge supercomputing technologies

The users of CSCS

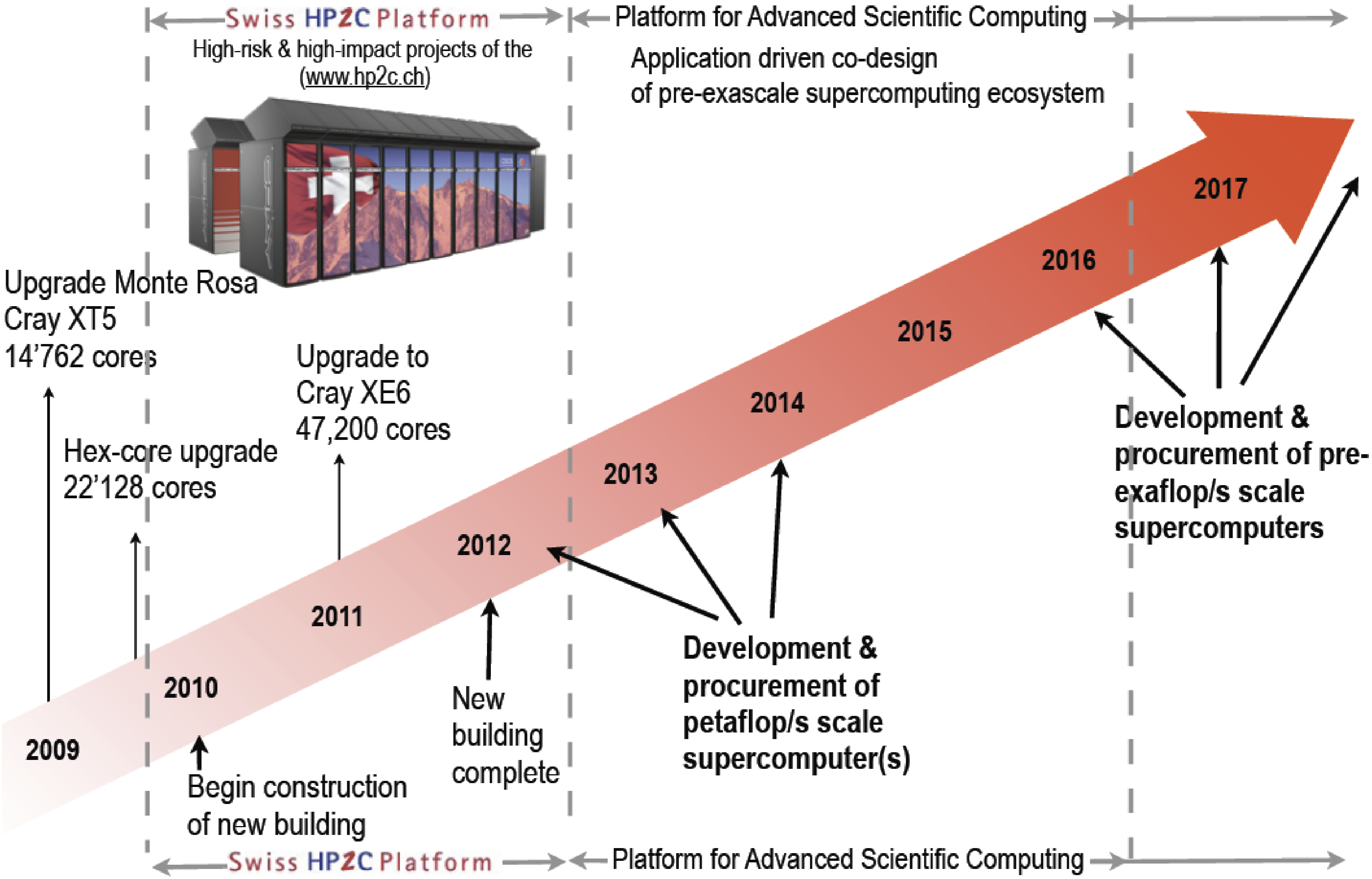
- **Scientific users can access CSCS Computing resources for free**
  - They have to submit project requests that are assessed by international experts
  - 450 million computing hours have been allocated in 2013
  - 80 projects, over a 1000 users



The office building

The computer building

The computer building: machine room


Swiss HP2C Platform
High-risk & high-impact projects of the
(www.hp2c.ch)
Platform for Advanced Scientific Computing
Application driven co-design
of pre-exascale supercomputing ecosystem
Upgrade Monte Rosa
Cray XT5
14'762 cores
Hex-core upgrade
22'128 cores
Upgrade to
Cray XE6
47,200 cores
2009
2010
2011
2012
2013
2014
2015
2016
2017
Begin construction
of new building
New
building
complete
Development &
procurement of
petaflop/s scale
supercomputer(s)
Development &
procurement of pre-
exaflop/s scale
supercomputers
Swiss HP2C Platform
Platform for Advanced Scientific Computing

HP2C

The High Performance and High Productivity Computing Platform

2009-13

Scientific Problem

Domain science projects lead by research groups at Swiss universities

Supercomputer

Simulations + Theory + Experiment

Swiss Universities / Federal Institutes of Technology
(presently **12 domain science projects** in HP2C Platform)

Interdisciplinary teams consisting of:
> model & method development
> application software design / engineering
> system software (everything between apps & hardware)
> numerical libraries / programming environments
> mapping methods onto computer hardware/ systems
> hardware design / engineering

CSCS & University della Svizzera italiana
(collaboration with computer industry: e.g. Cray, IBM, Mellanox, SCS)

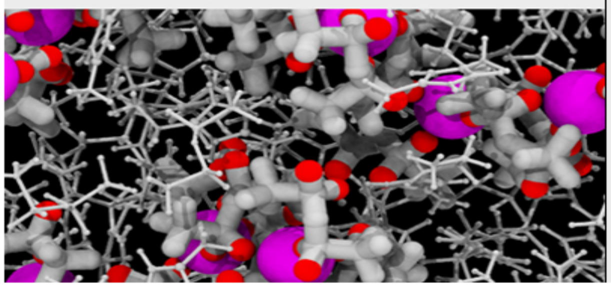
IT manufacturers – system integrators

Swiss Platform for Advanced Scientific Computing (PASC)

pasc
Platform for Advanced Scientific Computing

ABOUT | NEWS | NETWORKS | PROJECTS | ACTIVITIES | CONTACTS

Materials Simulations Network



Events

Platform of Advanced Scientific Computing Conference
14.10.2013

The first Platform of Advanced Scientific Computing Conference (PASC14) will take place on June 2...

Latest News

Additional Co-Design Projects accepted
10.01.2014

2014 Call for Co-Design Projects
10.01.2014

Welcome to the Swiss **Platform for Advanced Scientific Computing** (PASC) - PASC is a structuring project jointly supported by the Swiss University Conference (SUC) and the Council of Federal Institutes of Technology (ETH Board).

PASC is coordinated by the Università della Svizzera italiana (USI) in collaboration with CSCS, the Swiss National Supercomputing Centre of the ETH Zurich, and with the other Swiss universities and the EPF Lausanne.

The platform's overarching goal is to position Swiss computational sciences in the emerging exascale-era. It is complementary to the supercomputing-hardware-focused elements of the Swiss High-Performance and Networking (HPCN) initiative. The PASC consolidates and builds on the achievements of the current High-Performance and High-Productivity Computing (HP2C) project which supported 13 large-scale projects in the period 2009-2013.

PASC aims to promote joint effort to address key scientific issues in different domain sciences through interdisciplinary collaborations between domain scientists, computational scientists, software developers, computing centres and hardware developers. Thus, PASC builds on the principle of co-design, namely that software codes exploiting the potential of the next generation of computing architectures need to be jointly and interactively developed by these actors throughout the whole value chain.

SUK·CUS
Swiss university conference

ETH BOARD

http://www.pasc-ch.org

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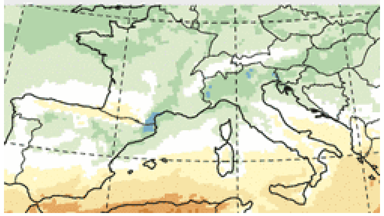
Platform for Advanced Scientific Computing

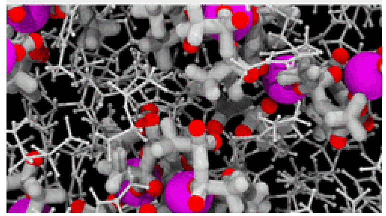
2013-16

Domain Science Networks

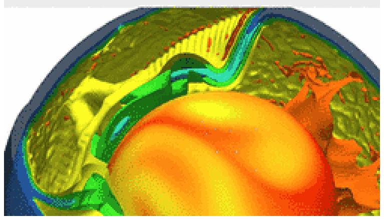
Climate Network



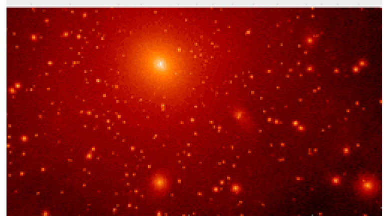
Materials Simulations Network



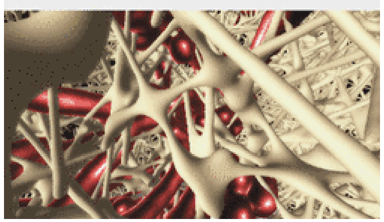
Solid Earth Dynamics Network



Physics Network



Life Sciences Network

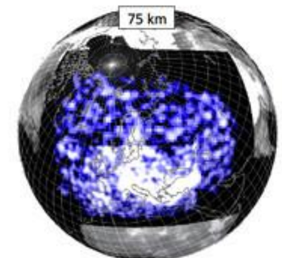


?????

Co-design Projects

GeoScale

A framework for multi-scale seismic modelling and inversion.



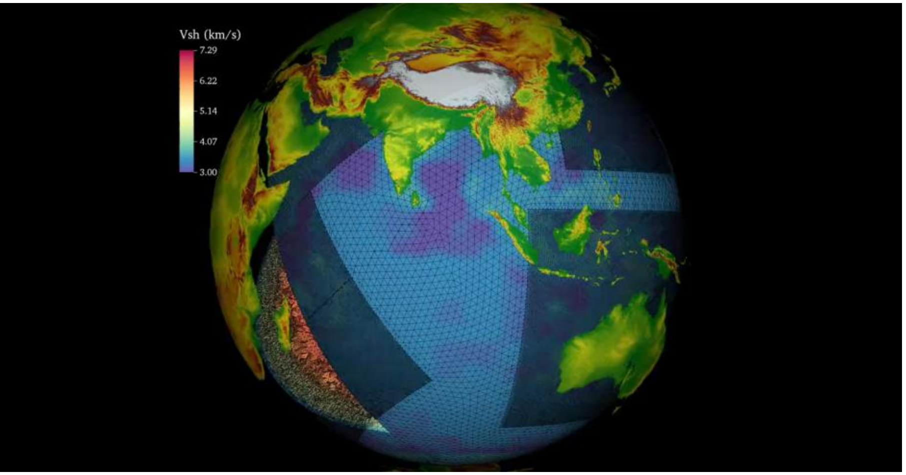
Co-Design Projects

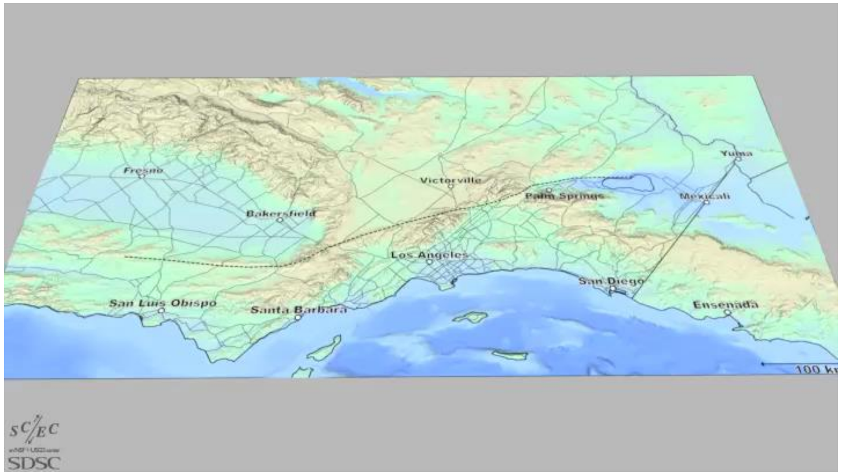
Projects | Call | Submission | HP2C

Select a project from the list below to get more information about the Co-design Projects supported by PASC.

Angiogenesis
Angiogenesis in Health and Disease: In-vivo and in-silico; PI: Petros Koumoutsakos (ETH Zurich)
DIAPHANE
A common platform for application-independent Radiative Transport in astrophysical simulations; PI: Lucio Mayer (University of Zurich)
Electronic Structure Calculations
Reduced scaling electronic structure calculations based on a versatile library for sparse matrix multiplication; PI: Jürg Hutter (University of Zurich)
ENVIRON
A Library for Complex Electrostatic Environments in Electronic-structure Simulations; Stefan Goedecker (University of Basel)
Genomic Data Processing
Portable Scalable Concurrency for Genomic Data Processing; PI: Ioannis Xenarios (University of Lausanne)
GeoPC
Infrastructure development for hybrid parallel smoothers for multigrid preconditioners; PI: Paul Tackley (ETH Zurich)
GeoScale
A framework for multi-scale seismic modelling and inversion; PI: Andreas Fichtner (ETH Zurich)
Grid Tools
Towards a library for hardware oblivious implementation of stencil based codes; PI: Oliver Fuhrer (Meteosuisse)
Heterogeneous Compiler Platform
Heterogeneous Compiler Platform for Advanced Scientific Codes; PI: Torsten Hoefler (ETH Zurich)
HPC-ABGEM
High-performance computing tools for agent-based general ecosystems models (HPC-ABGEM); PI: Christoph Zollikofer (University of Zurich)

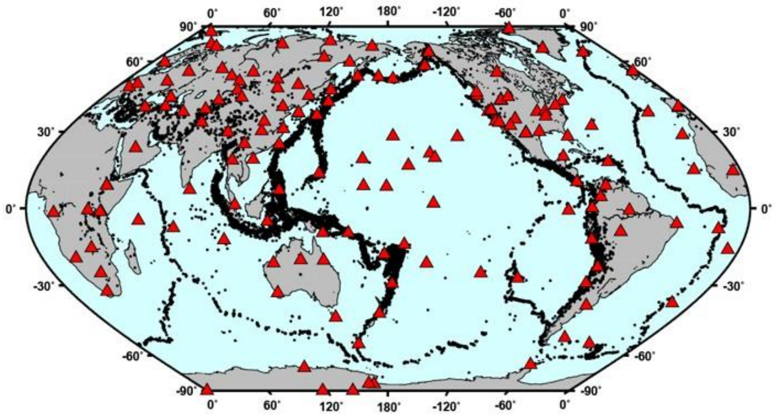
Geoscale project (ETHZ, USI, CSCS)

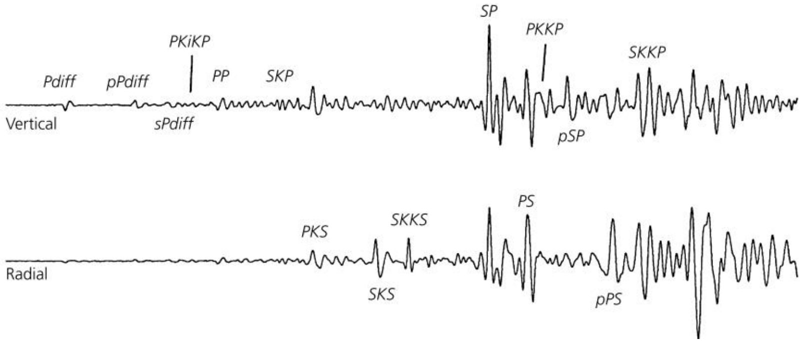




Earth models for seismic (compressional/shear) velocities

Seismicity and seismometers





What is a supercomputer?

What is a supercomputer?

- **A supercomputer performs a huge number of mathematical operations in parallel**
- **The computing power is expressed in**
  - FLOPS (Floating Point Operations) per second
- **The Piz Daint supercomputer at CSCS has a computing power of**
  - 6.767 PFlops = 6.767 x 10^{15} = 6.702 Quadrillion of mathematical operations per second
  - Piz Daint can compute in **one day** more than a modern laptop could compute in **941 years**

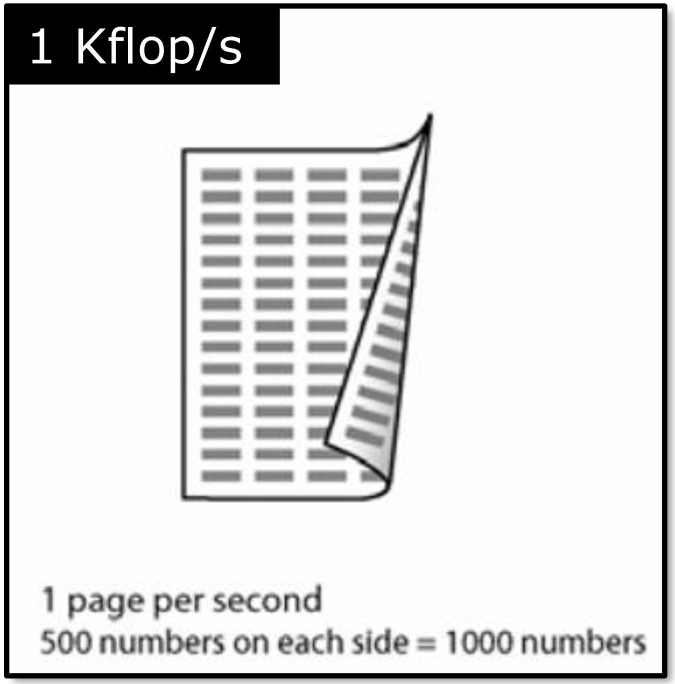
Units of Measure in Computing

- **High Performance Computing (HPC) units are:**
  - Flops: floating point operations
  - Flop/s: floating point operations per second
  - Bytes: size of data (double precision floating point number is 8)
- **Typical sizes are millions, billions, trillions…**

Mega	**Mflop/s** = 10^6 flop/sec	Mbyte = 10^6 byte
Giga	**Gflop/s** = 10^9 flop/sec	Gbyte = 10^9 byte
Tera	**Tflop/s** = 10^{12} flop/sec	Tbyte = 10^{12} byte
Peta	**Pflop/s** = 10^{15} flop/sec	Pbyte = 10^{15} byte
Exa	**Eflop/s** = 10^{18} flop/sec	Ebyte = 10^{18} byte

Units of Measure in Computing

- **Let us say you can print:**
  5 columns of 100 number each; on both sides of the page = 1000 numbers (Kflop) in one second **(1 Kflop/s)**



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Units of Measure in Computing

- **Let us say you can print:**

  1000 pages about 10 cm = 10^6 numbers (Mflop)

  2 reams of paper per seconds **(1 Mflop/s)**

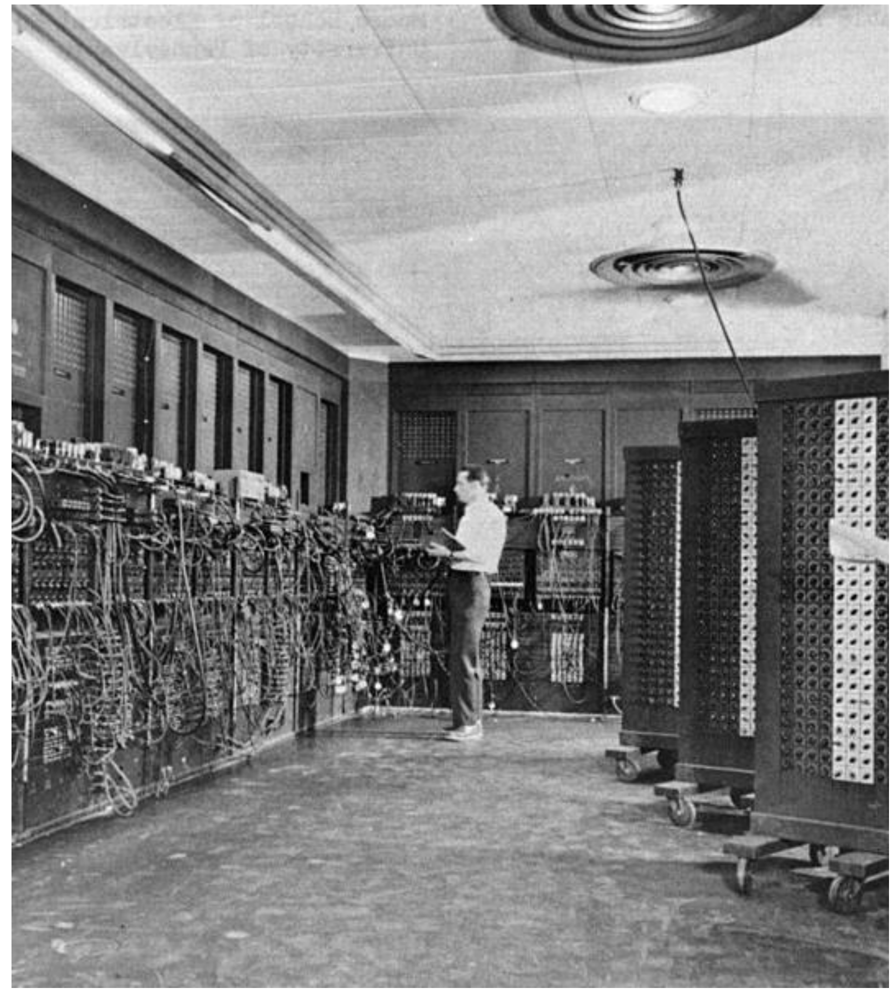
Units of Measure in Computing

- **Let us say you can print:**
  10^{15} numbers (Pflop) = 100,000 km
  (1/4 distance to the moon) stack printed per second **(1Pflop/s)**

Electronic Numerical Integrator And Computer

ENIAC, USA, 1946

- **Ballistic Calculations**
- **Size**
  - 27 t
  - 2.4 m × 0.9 m × 30 m
  - 150 kW
- **Cost:**
  - $468’000 (1946)
  - $5’900’000
  - One multiplication ~2.8 ms



Earth Simulator, Japan, 2002

- **Run global climate models**
- **Size**
  - Interconnect 14 m x 13 m
  - Computer 41 m x 40 m
  - 6.4 MW
- **Cost $400,000,000**

35.86 TFLOPS

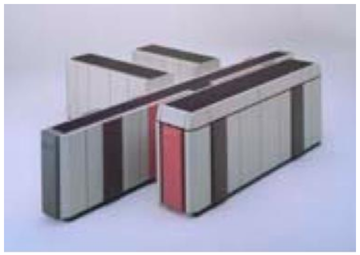
Cray XC30 „Piz Daint", Switzerland, 2014

- **User Lab for Swiss Scientists**
- **115‘984 cores - 272 TB of RAM**
- **4PB TB local disks**

- **Size**
  - 23 t
  - 47 m^2
  - 2,325 MW

6,700 PFlops

Short life cycle of about 3 years



1991 NEC SX3
5.5 GF Adula

1996 NEC SX4
10 GF Gottardo

1999 NEC SX5
64 GF Prometeo

2002 IBM SP4
1.3 TF Venus

2005 Cray XT3
5.8 TF Palu

2006 IBM P5
4.5 TF Blanc

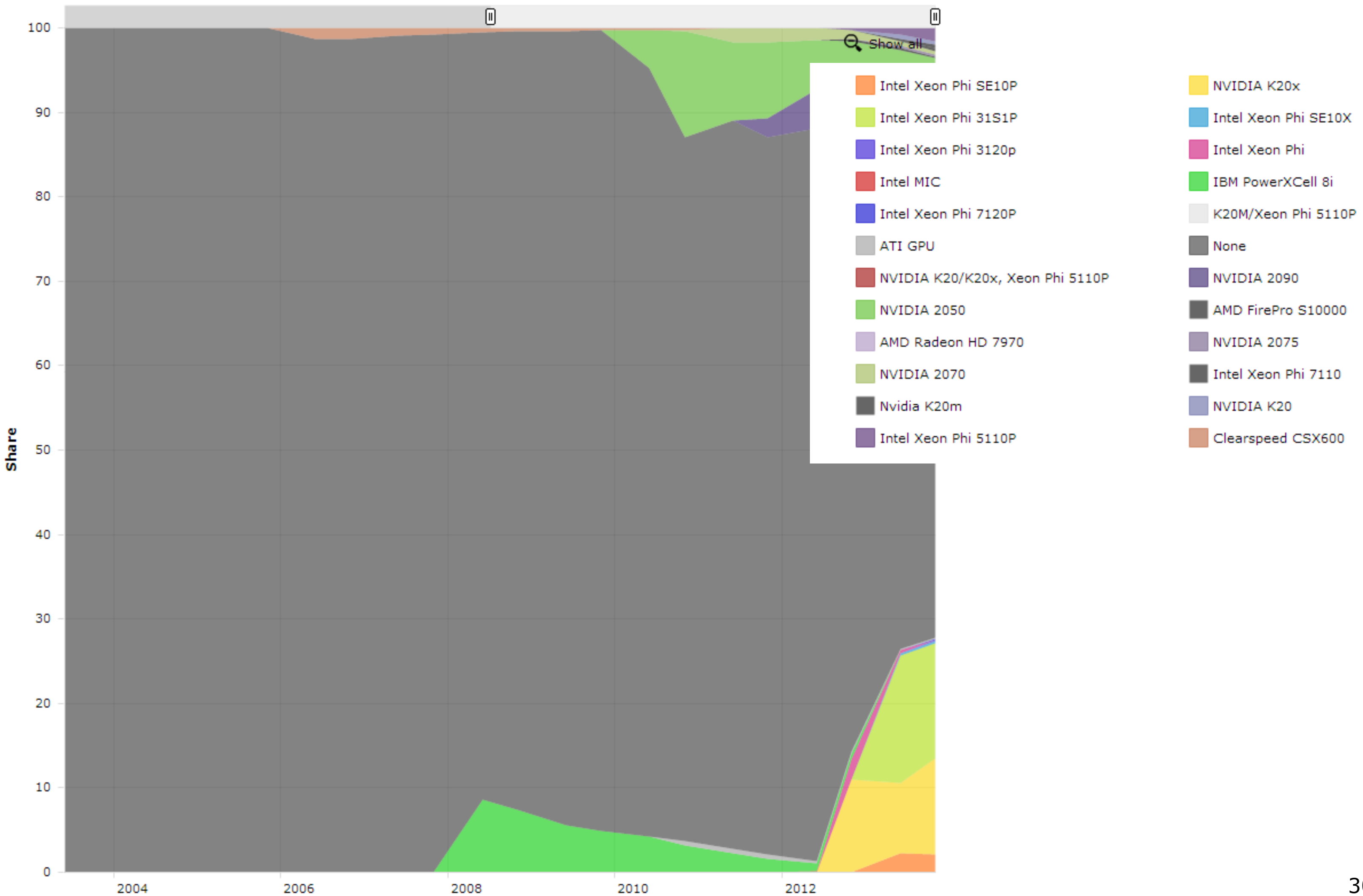
2009-12 Cray XE6
402 TF Monte Rosa

2013 Cray XC30
6.750 PF Piz Daint

TOP 500 List of Supercomputers

Rank	Site	System	Cores	Rmax in Tflops/s	Rpeak in Tflops/s	Power (KW)
1	National Super Computer Center China	**Tianhe-2 (MilkyWay-2)** - Intel Xeon Intel Xeon Phi	3,120,000	33,862.7	54,902.4	17,808
2	DOE/SC/Oak Ridge United States	**Titan** - Cray XK7 Opteron + NVIDIA K20x	560,640	17,590.0	27,112.5	8,209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQ, IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN, Japan	K computer, SPARC64 Fujitsu	705,024	10,510.0	11,280.4	12,660
5	DOE/SC/Argonne United States	**Mira** - BlueGene/Q, IBM	786,432	8,586.6	10,066.3	3,945
6	CSCS, Switzerland	**Piz Daint** - Cray XC30, Intel Xeon , NVIDIA K20x	115,984	6,271.0	7,788.9	2,325
7	Texas Advanced Computing Center, US	**Stampede** - Intel Xeon, Intel Xeon Phi, Dell	462,462	5,168.1	8,520.1	4,510
8	Forschungszentrum Juelich (FZJ), Germany	**JUQUEEN** - BlueGene/Q, IBM	458,752	5,008.9	5,872.0	2,301
9	DOE/NNSA/LLNL United States	**Vulcan** - BlueGene/Q, IBM	393,216	4,293.3	5,033.2	1,972
10	Leibniz Rechenzentrum Germany	**SuperMUC** - Xeon E5-2680 IBM	147456	2,897.0	3,185.1	3,423

Accelerators / Development over time



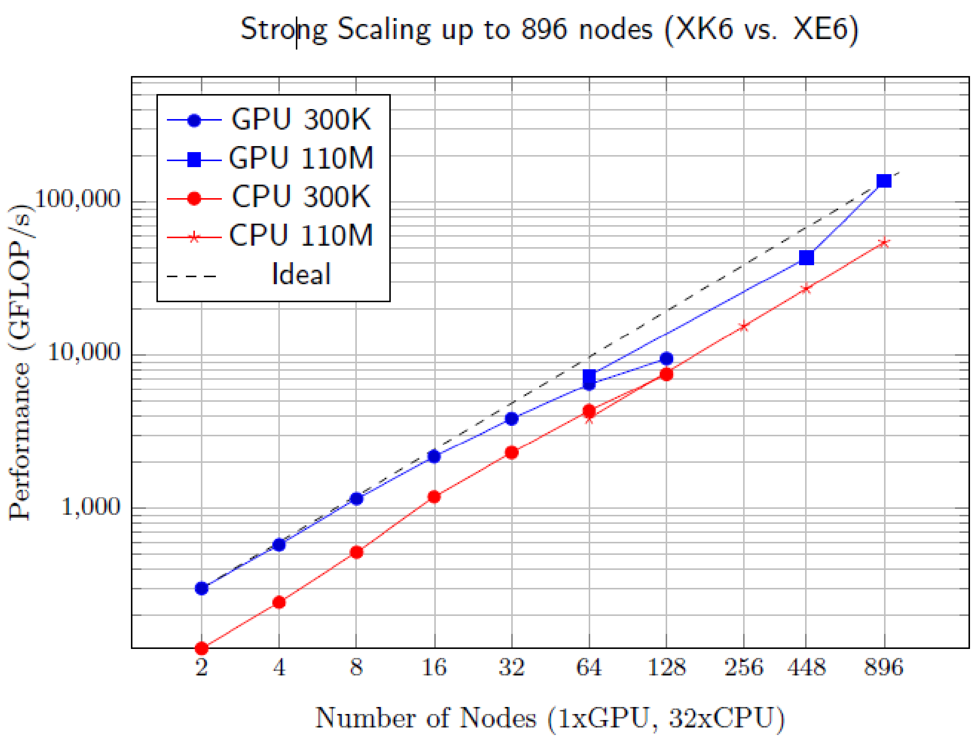
What is changing in supercomputing due to accelerators?

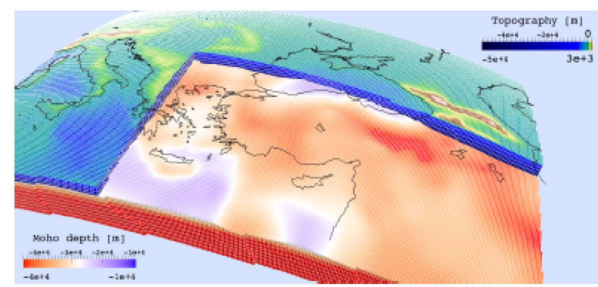
HP2C Project: GPU Version of SPECFEM3D

- **SPECFEM3D** is a higher-order finite element code that simulates elastic/acoustic waves on arbitrary hexahedral meshes.
- Written using Fortran90 and MPI
- Excellent performance and scalability (> 90%)
- Large user community across large array of applications
- **GPU Code** for **forward** and **adjoint** system with SPECFEM3D.
- Seismic imaging via adjoint methods

HP2C: Strong Scaling for Case Study Turkey Earthquakes

- 19M mesh covering Europe, Middle East/Northern Africa.





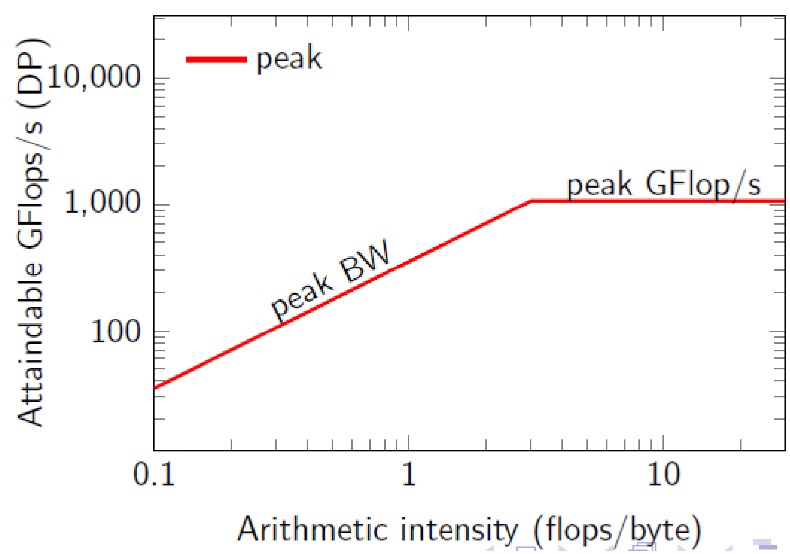
- Similar excellent performance on future manycore architectures? --> **Roofline Model**

Roofline Model

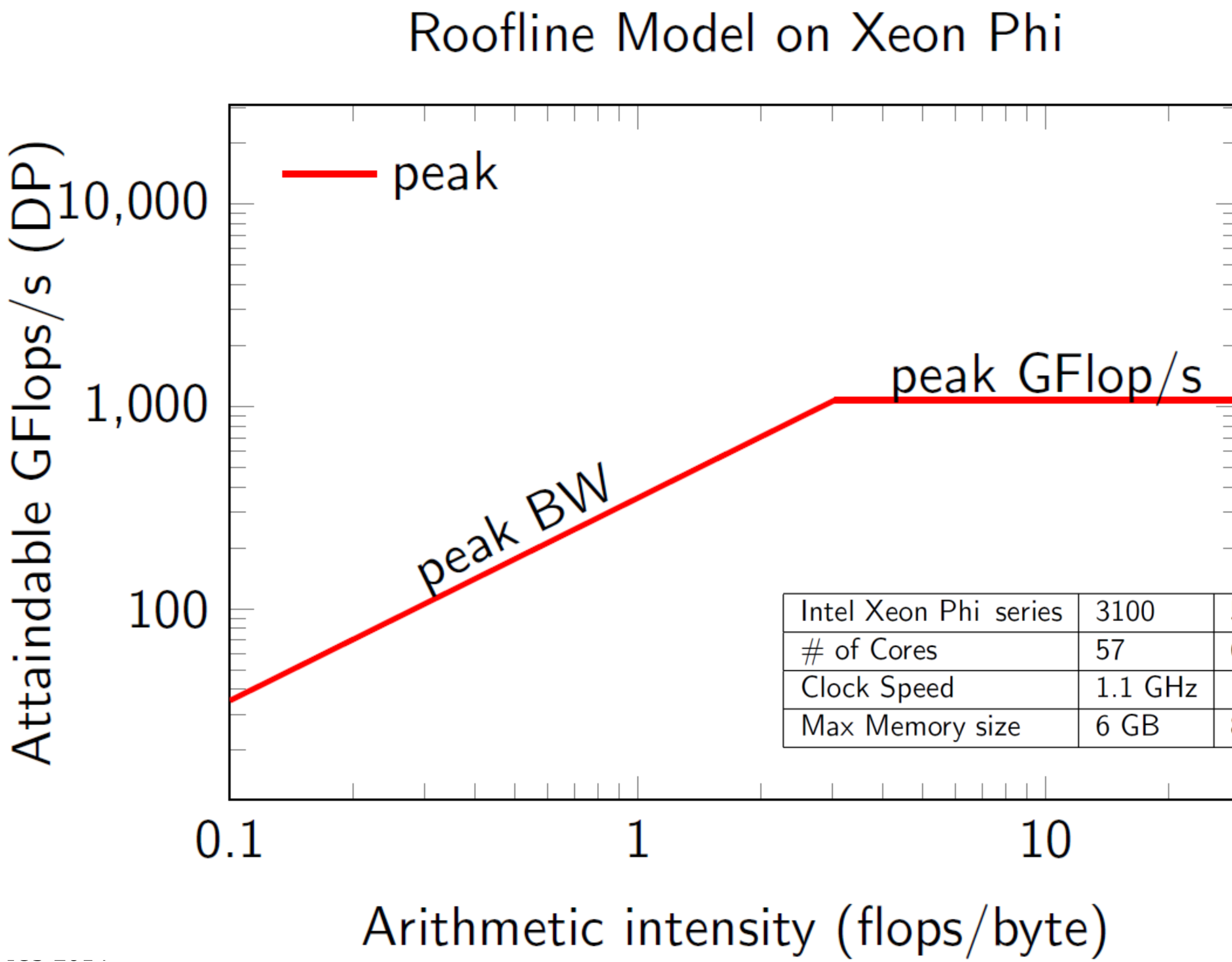
- **Arithmetic intensity**: $q = \dfrac{\text{floating-point operations}}{\text{byte off-chip memory traffic}}$
- High $q \rightarrow$ compute bound (dense algebra, FFT, ...)
- Low $q \rightarrow$ bandwidth bound (sparse algebra, stencils, ...)
- Performance Gflop/s = min(Peak Gflop/s, Stream BW$\times q$)
- Roofline gives upperbound for performance for given q

The Roofline Model: A pedagogical tool for program analysis and optimization (Williams, Patterson, 2008)

Roofline Model on Xeon Phi

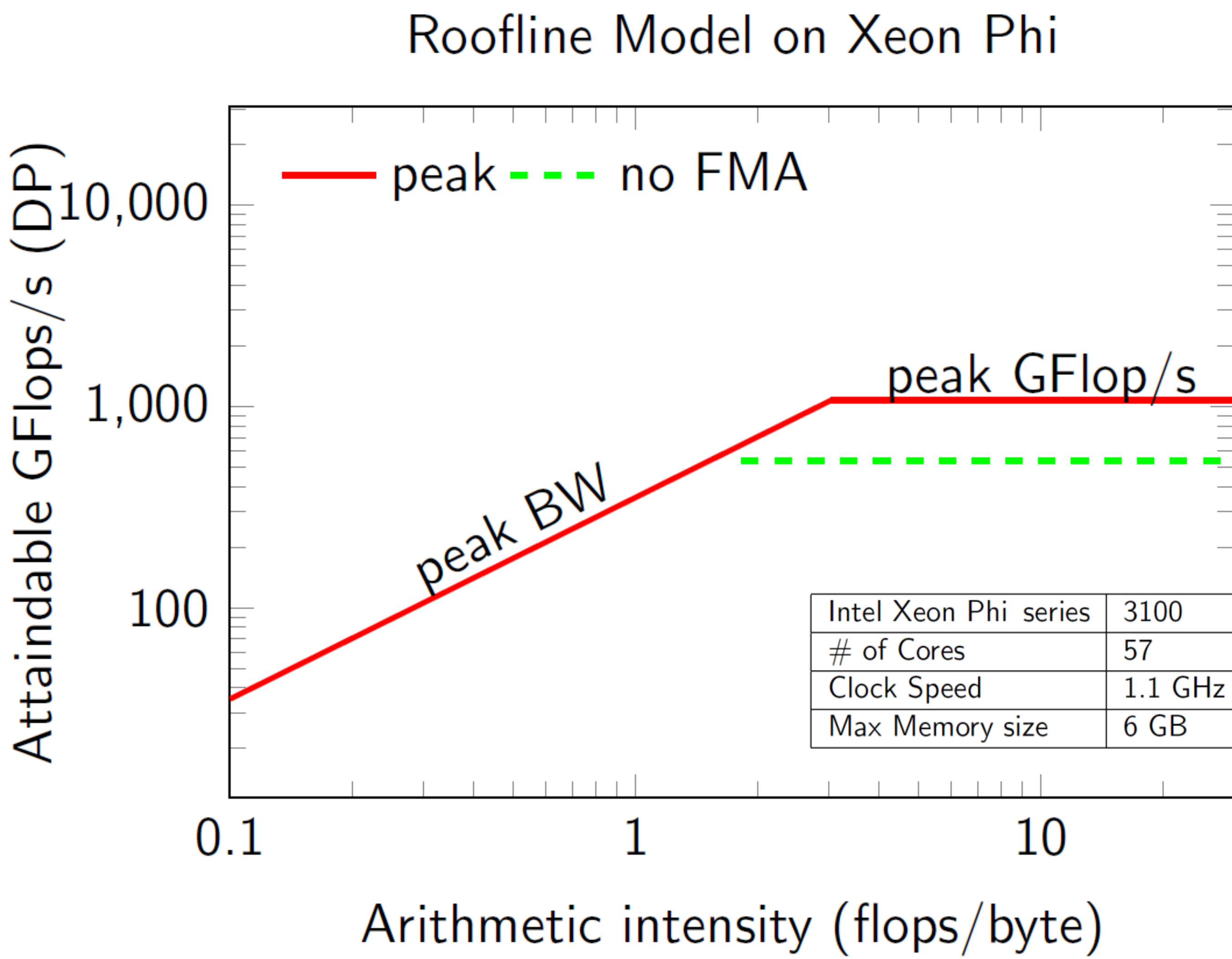


Roofline Model on Intel Xeon Phi



Intel Xeon Phi series	3100	5100	7100
# of Cores	57	60	61
Clock Speed	1.1 GHz	1.053 GHz	1.238 GHz
Max Memory size	6 GB	8 GB	16 GB

Roofline Model on Intel Xeon Phi



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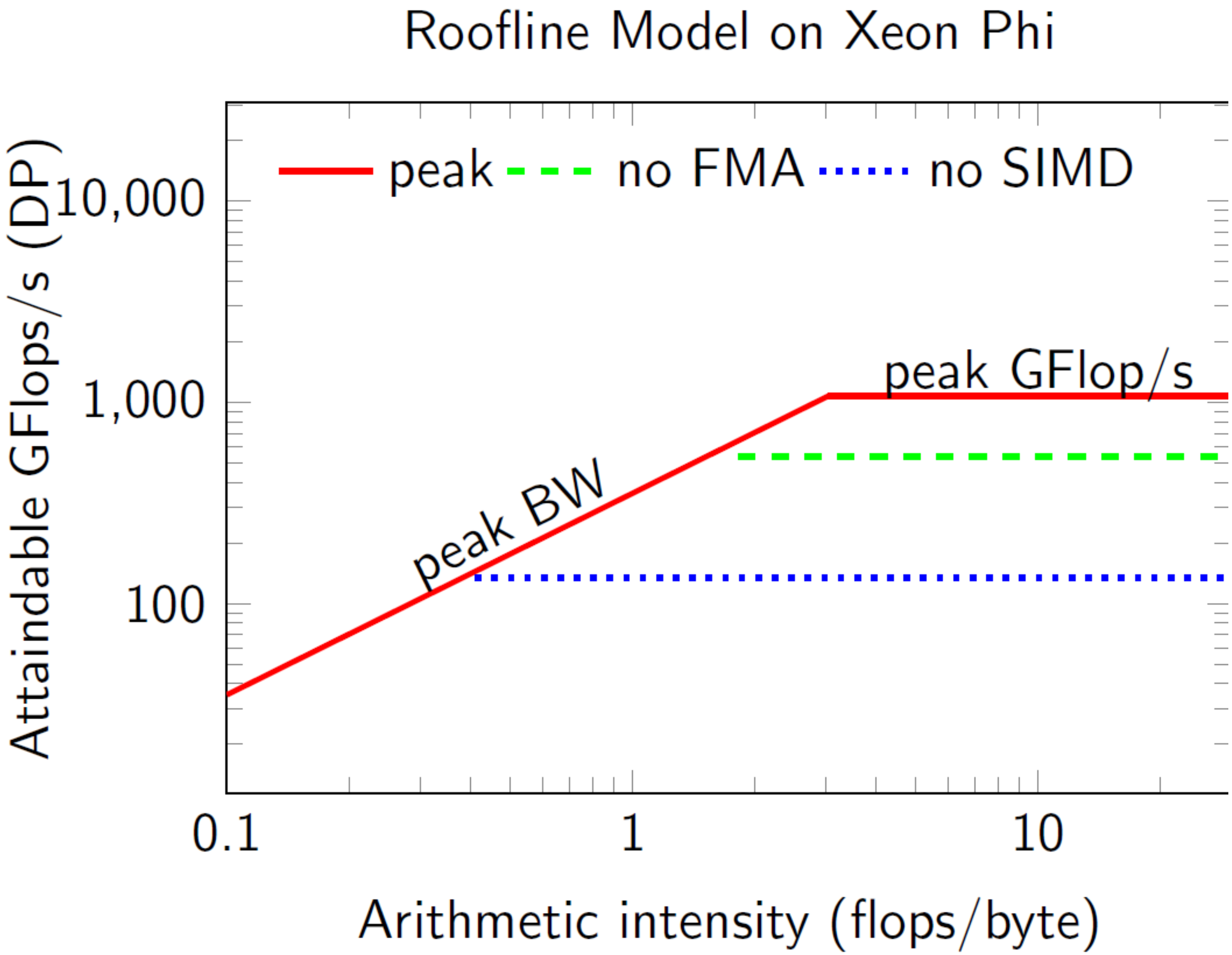

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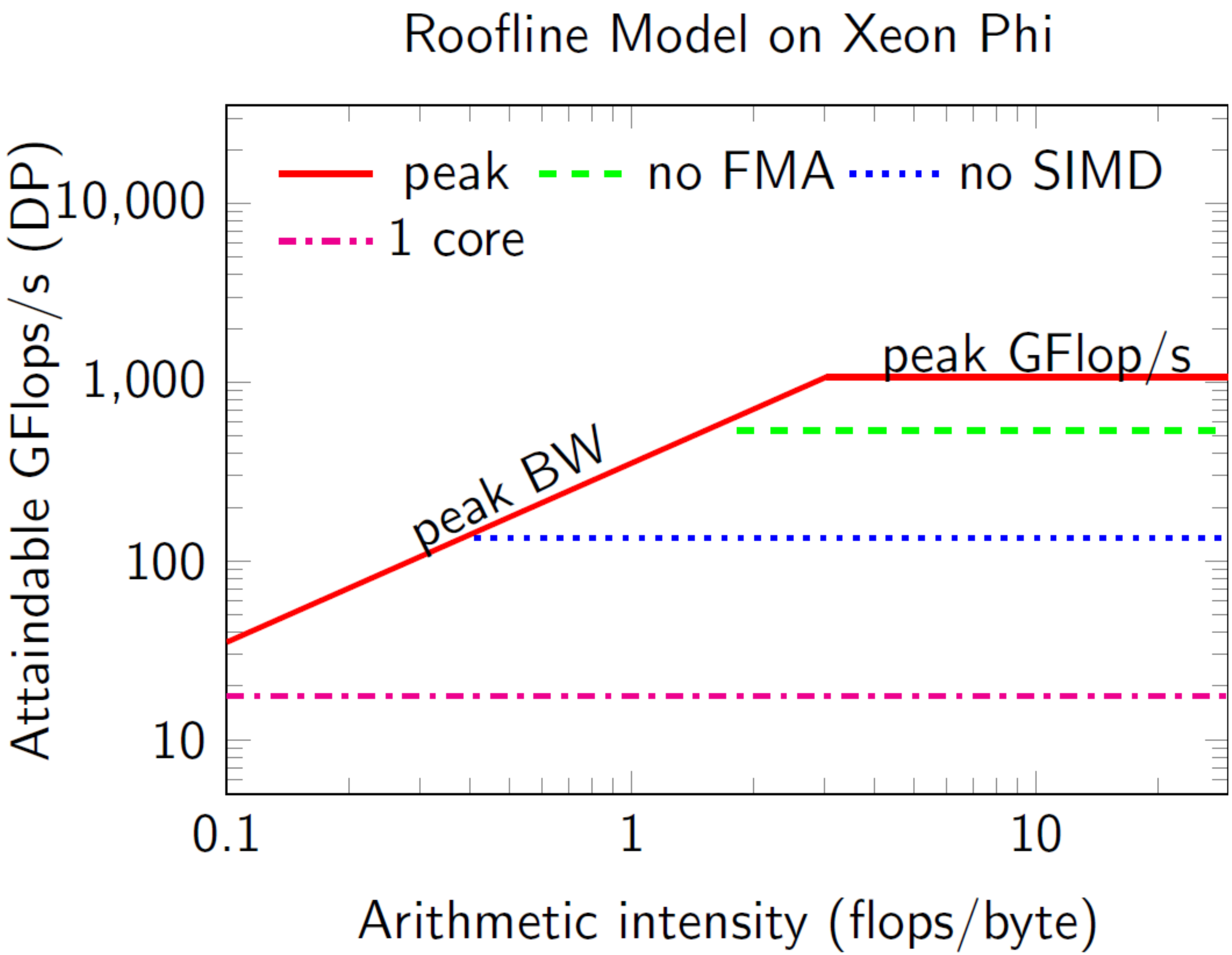

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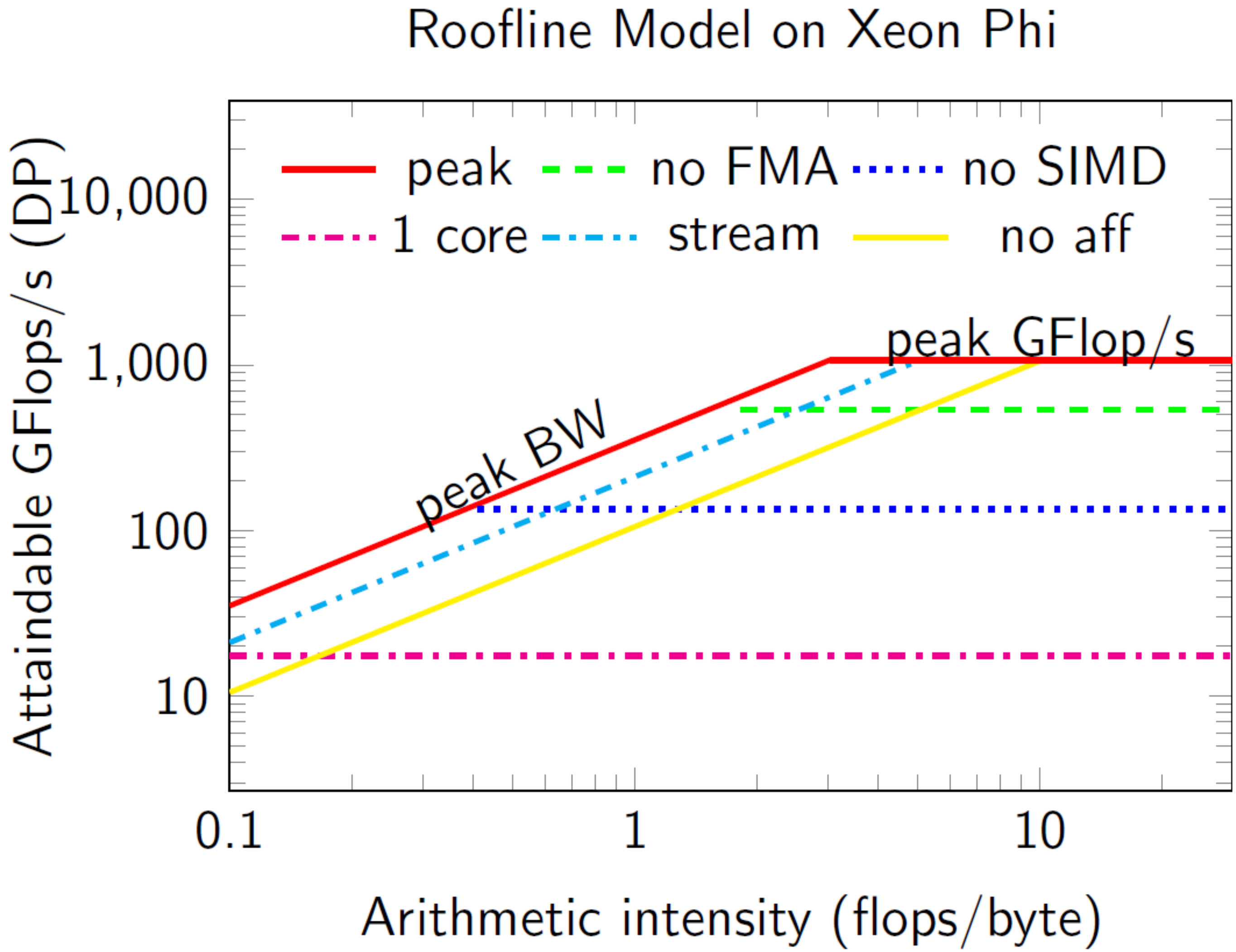
Roofline Model on Intel Xeon Phi



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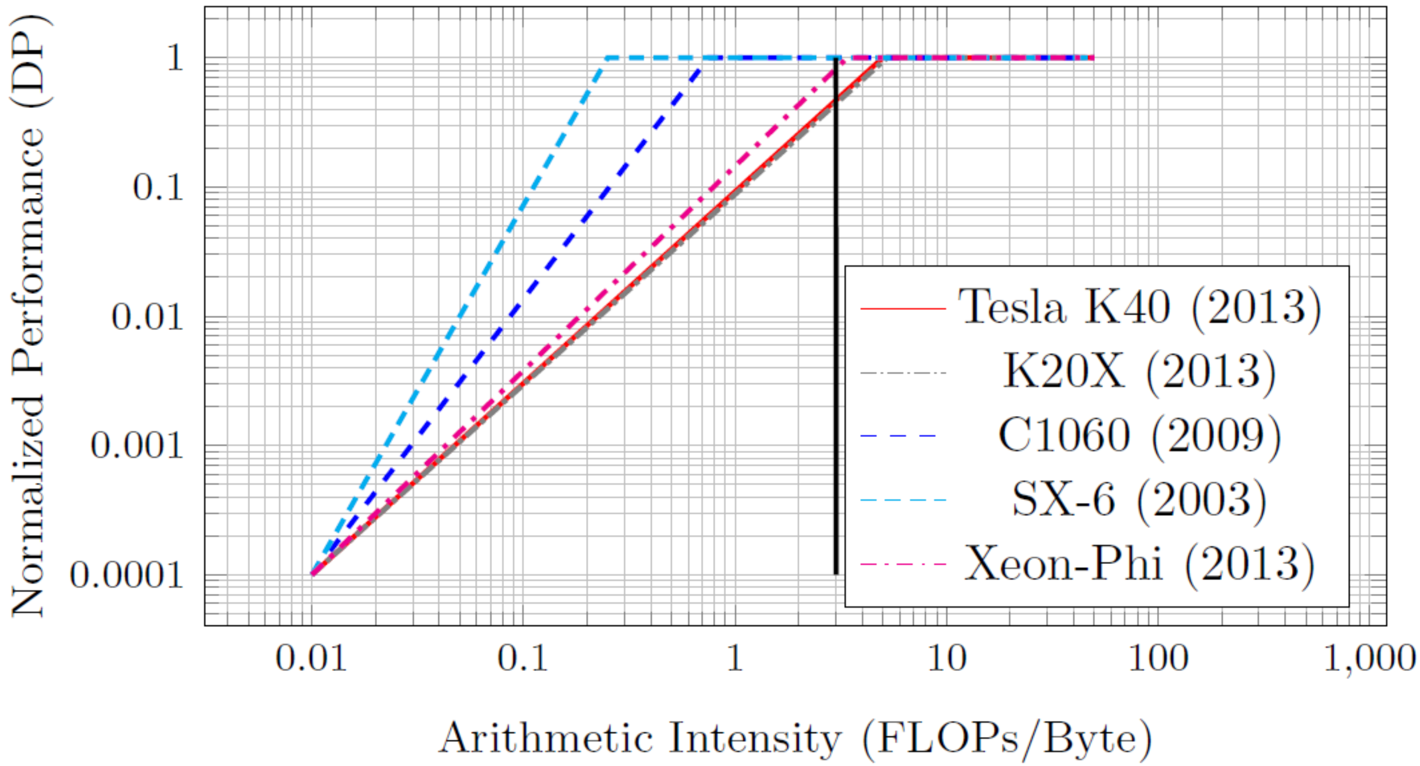
SPECFEM and Roofline Trend Model (2003-2014)



- Arithmetic intensity for Peak: 0.25(2003), 0.8(2009), 6.2 (2013)
- **Re-design/Co-design algorithms** to increase **arithmetic intensity** on **manycores/accelerators.**

Interior-point methods for large scale stochastic optimization on high-performance computers

Inequality constrained minimization

Inequality constrained minimization

$$\min_{\mathbf{x},\mathbf{x_0}} f_0(\mathbf{x}, \mathbf{x}_0)$$
$$\text{s.t. } f_i(\mathbf{x}, \mathbf{x}_0) \geq 0, \quad i = 1, \dots, m$$
$$A(\mathbf{x}_0) \cdot \mathbf{x} = b_j, \quad j = 1, \dots, N_e$$

with f_i **nonconvex**, twice continuously differentiable, $A(x_0)$ full rank, $\mathbf{x}_0$ control variables, $\mathbf{x}$ state variables.

Ongoing project:

- Exploiting structure in very large-scale **interior-point optimization**
- Software to solve QPs or NLPs on massively-parallel computers
- DOE INCITE projects on "Titan" (100M CPU h on Cray XK7) and "Mira" (BG/Q)
- 1.95 billion uncertain parameters, 1.94 billion constraints, 25K control variables on "Titan" under "real-time" constraints (30 min).

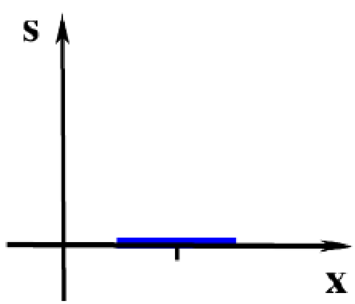
First Order Optimality Conditions

Simplex Method:

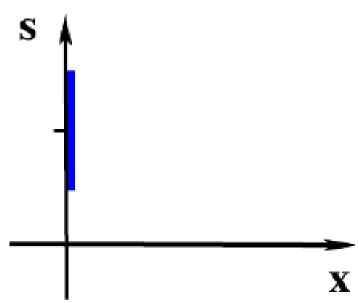
$$
\begin{aligned}
Ax &= b \\
A^T y + s &= c \\
XSe &= 0 \\
x, s &\geq 0
\end{aligned}
$$

Interior Point Method:

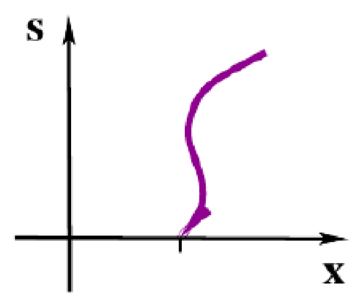
$$
\begin{aligned}
Ax &= b \\
A^T y + s &= c \\
XSe &= \mu e \\
x, s &\geq 0
\end{aligned}
$$



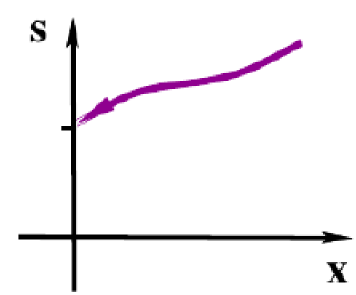
Basic: x > 0, s = 0



Nonbasic: x = 0, s > 0



"Basic": x > 0, s = 0



"Nonbasic": x = 0, s > 0

Nocedal, Wright, **Numerical Optimization**, Springer, 2006.

Convergence of IPM

Scenarios	Variables	Number of IPM Iterations standard	correctors	warm-started
100	105K	23	20	7
200	209K	64	25	9
800	836K	28	22	11
1200	1.6M	33	26	12
2400	3.1M	29	21	9

Theory IPM converge in $O(\sqrt{n})$ iterations

Practise IPM converge in $O(1)$ to $O(log\ n)$ iterations

. . . but one iteration may be VERY expensive

(Slide Source: J. Gondzio, School of Mathematics, University of Edinburgh)

KKT systems in IPMs for LP, QP, and NLP

LP
$$\begin{pmatrix} \Theta^{-1} & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \begin{pmatrix} f \\ d \end{pmatrix}$$

QP
$$\begin{pmatrix} Q + \Theta^{-1} & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \begin{pmatrix} f \\ d \end{pmatrix}$$

NLP
$$\begin{pmatrix} Q(x,y) + \Theta_P^{-1} & A^T \\ A & -\Theta_D^{-1} \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \begin{pmatrix} f \\ d \end{pmatrix}$$

$\rightarrow$ another regularization is related to Hessian modification

Stochastic optimization problems

Inequality constrained minimization

$$\begin{aligned} \min_{\mathbf{x},\mathbf{x_0}} \ & f_0(\mathbf{x}, \mathbf{x}_0) \\ \text{s.t.} \ & f_i(\mathbf{x}, \mathbf{x}_0) \geq 0, \quad i = 1, \dots, m \\ & A(\mathbf{x}_0) \cdot \mathbf{x} = b_j, \quad j = 1, \dots, N_e \end{aligned}$$

with f_i nonconvex, twice continuously differentiable, $A(x_0)$ full rank.

Basic stochastic programming

$$\begin{aligned} \min_{\mathbf{x},\mathbf{x_0}} \ & F_0(\mathbf{x}, \mathbf{x}_0) = \mathbb{E}[f_0(\mathbf{x}, \mathbf{x}_0, \xi)] \\ \text{s.t.} \ & F_i(\mathbf{x}, \mathbf{x}_0) = \mathbb{E}[f_i(\mathbf{x}, \mathbf{x}_0, \xi)] \geq 0, \quad i = 1, \dots, m \\ & F_j(\mathbf{x}, \mathbf{x}_0) = \mathbb{E}[A(\mathbf{x}_0, \xi)\mathbf{x} = b_j(\xi)], \quad j = 1, \dots, N_e \end{aligned}$$

with variables $(\mathbf{x}, \mathbf{x}_0)$, problem data are f_i nonconvex, random distribution of ξ, A full rank.

Example: Two-stage stochastic optimization problems

$$\min_{\mathbf{x},\mathbf{x}_0} \left(\frac{1}{2}\mathbf{x}_0{}^T Q_0 \mathbf{x}_0 + c_0^T \mathbf{x}_0\right) + \mathbb{E}_\xi[G(\mathbf{x},\mathbf{x}_0,\xi)]$$
$$\text{s.t.} \quad T_0\mathbf{x}_0 = b_0, \mathbf{x}_0 \geq 0,$$

where the recourse function $G(\mathbf{x}_0, \xi)$ is defined by

$$G(\mathbf{x},\mathbf{x}_0,\xi) = \min_{\mathbf{x}} \frac{1}{2}\mathbf{x}^T Q_\xi \mathbf{x} + c_\xi^T \mathbf{x}$$
$$\text{s.t.} \quad T_\xi \mathbf{x}_0 + W_\xi \mathbf{x} = b_\xi, \mathbf{x} \geq 0.$$

- Matrices Q_ξ and W_ξ have full row rank.
- $\mathbf{x}_0$ is called the *control*, which is a decision to be made now.
- The *state* $\mathbf{x}$ is a corrective decision that one makes in the future after some random event occurs.
- The stochastic optimization problem finds the optimal control to be made now that has the minimal expected cost in the future.

Example: Stochastic optimization problems

$$\min_{\mathbf{x},\mathbf{x}_0} \left(\frac{1}{2}\mathbf{x}_0{}^T Q_0 \mathbf{x}_0 + c_0^T \mathbf{x}_0 \right) + \mathbb{E}_\xi[G(\mathbf{x}, \mathbf{x}_0, \xi)]$$
$$\text{s.t. } T_0 \mathbf{x}_0 = b_0, \mathbf{x}_0 \geq 0,$$

where the recourse function $G(\mathbf{x}_0, \xi)$ is defined by

$$G(\mathbf{x}, \mathbf{x}_0, \xi) = \min_{\mathbf{x}} \frac{1}{2}\mathbf{x}^T Q_\xi \mathbf{x} + c_\xi^T \mathbf{x}$$
$$\text{s.t. } T_\xi \mathbf{x}_0 + W_\xi \mathbf{x} = b_\xi, \mathbf{x} \geq 0.$$

- Sample average approximations (SAAs): $\mathbb{E}_\xi = \frac{1}{N}\sum_{i=1}^N G(\mathbf{x}_0, \mathbf{x}, \xi_i)$
- SAA approach replaces the expectation $\mathbb{E}_\xi$ with the sample average $\sum_{i=1}^N G(\mathbf{x}_0, \mathbf{x}, \xi_i)$ computed by generating N samples $(Q_i, c_i, T_i, W_i, b_i)$ of ξ_i.

Large-scale (dual) block-angular QP/NLP

$$
\begin{array}{llllll}
\min\limits_{x_i} & \frac{1}{2}\mathbf{x}_0{}^T Q_0 \mathbf{x}_0 + c_0^T \mathbf{x}_0 + \frac{1}{N}\sum_{i=1}^{N}\left(\frac{1}{2}x_i{}^T Q_i x_i + c_i{}^T x_i\right) \\
\text{s.t.} & T_0\mathbf{x}_0 & & & & = b_0, \\
& T_1\mathbf{x}_0 + & W_1 x_1 & & & = b_1, \\
& T_2\mathbf{x}_0 + & & W_2 x_2 & & = b_2, \\
& \vdots & & & \ddots & \vdots \\
& T_N\mathbf{x}_0 + & & & W_N x_N & = b_N, \\
& \mathbf{x}_0 \geq 0, & x_1 \geq 0, & x_2 \geq 0, & \ldots, & x_N \geq 0.
\end{array}
$$

In terminology of stochastic QPs/NLPs:

1. First-stage variables (decision variables): $\mathbf{x}_0$
2. Second-stage variables (state variables): $x_1, \ldots, x_N$
3. Each diagonal block is a realization of a random scenario

$\longrightarrow$ interior-point solvers for structure QP/NLPs.

Linear algebra of primal-dual interior-point methods (IPM)

Convex quadratic problem

$$\begin{aligned} &\min \frac{1}{2} x^T Q x + c^T x \\ &\text{s.t.} Ax = b \\ &\quad x > 0 \end{aligned}$$

IPM Linear System

$$\begin{pmatrix} Q + \Delta & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

- Multi-stage stage stochastic programming
- nested arrow-shaped linear system (modulo a permutation)
- N is the number of scenarios

$$\begin{pmatrix}
Q_1 & W_1^T & & & & & & 0 & 0 \\
W_1 & 0 & & & & & & T_1 & 0 \\
& & Q_2 & W_2^T & & & & 0 & 0 \\
& & W_2 & 0 & & & & T_2 & 0 \\
& & & & \ddots & & & \vdots & \vdots \\
& & & & & Q_N & W_N^T & 0 & 0 \\
& & & & & W_N & 0 & T_N & 0 \\
0 & T_1^T & 0 & T_2^T & \dots & 0 & T_N^T & Q_0 & W_0^T \\
0 & 0 & 0 & 0 & \dots & 0 & 0 & W_0 & 0
\end{pmatrix}$$

Parallel Solution Procedure for KKT System

N scenarios distributed across $\mathcal{P}$ processes. $\mathcal{N}_p$ is set of scenarios assigned to process $p \in \mathcal{P}$. Each process $p \in \mathcal{P}$ executes the following steps:

(factorization phase)

1.1. Factorize $L_i D_i L_i^T = K_i$ for each $i \in \mathcal{N}_p$.

1.2. Compute SC contribution $S_i = B_i^T K_i^{-1} B_i$ for each $i \in \mathcal{N}_p$.

1.3. Accumulate $C_p = -\sum_{i \in \mathcal{N}_p} S_i$. On process 1, let $C_1 = C_1 + K_0$.

2. Reduce SC matrix $C = \sum_{r \in \mathcal{P}} C_r$ to process 1.

3. Factorize SC matrix $L_c D_c L_c^T = C$ in process 1.

(solve phase)

4.1. Solve $w_i = L_i^{-T} D_i^{-1} L_i^{-1} r_i$ for each $i \in \mathcal{N}_p$.Compute $v_p = \sum_{i \in \mathcal{N}_p} B_i^T w_i$.

4.2. On process 1, let $v_1 = v_1 + r_0$.

5. Reduce $v_0 = \sum_{i \in \mathcal{N}_p} v_i$ to process 1.

6.1. Solve $\Delta z_0 = C^{-1} v_0 = L_c^{-T} D_c^{-1} L_c^{-1} v_0$ in process 1.

6.2. Process 1 broadcasts z_0 to all other processes.

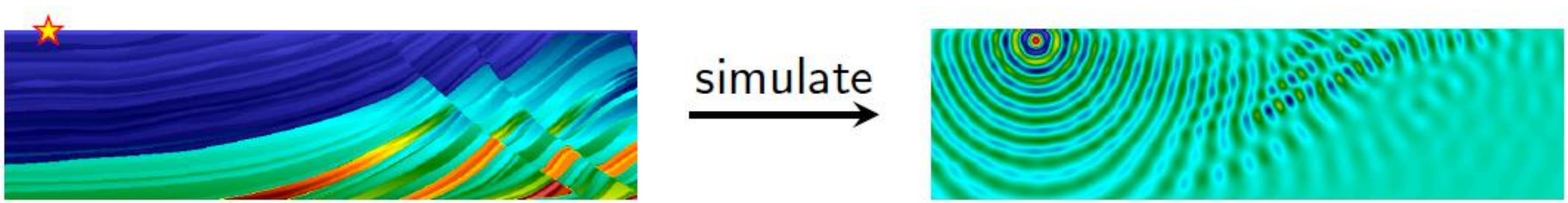
7. Solve $\Delta z_i = L_i^{-T} D_i^{-1} L_i^{-1}(B_i \Delta z_0 - r_i)$ for each $i \in \mathcal{N}_p$.

Application 3D Seismic Imaging (ETH, USI)

- Simulate subsurface wave y
- Helmholtz equation:

$$A(u, y) = -\mathbf{grad} \cdot (u(x)^2 \mathbf{grad}\, y(x)) - \omega^2 y(x) - f(x) = 0 \qquad (1)$$

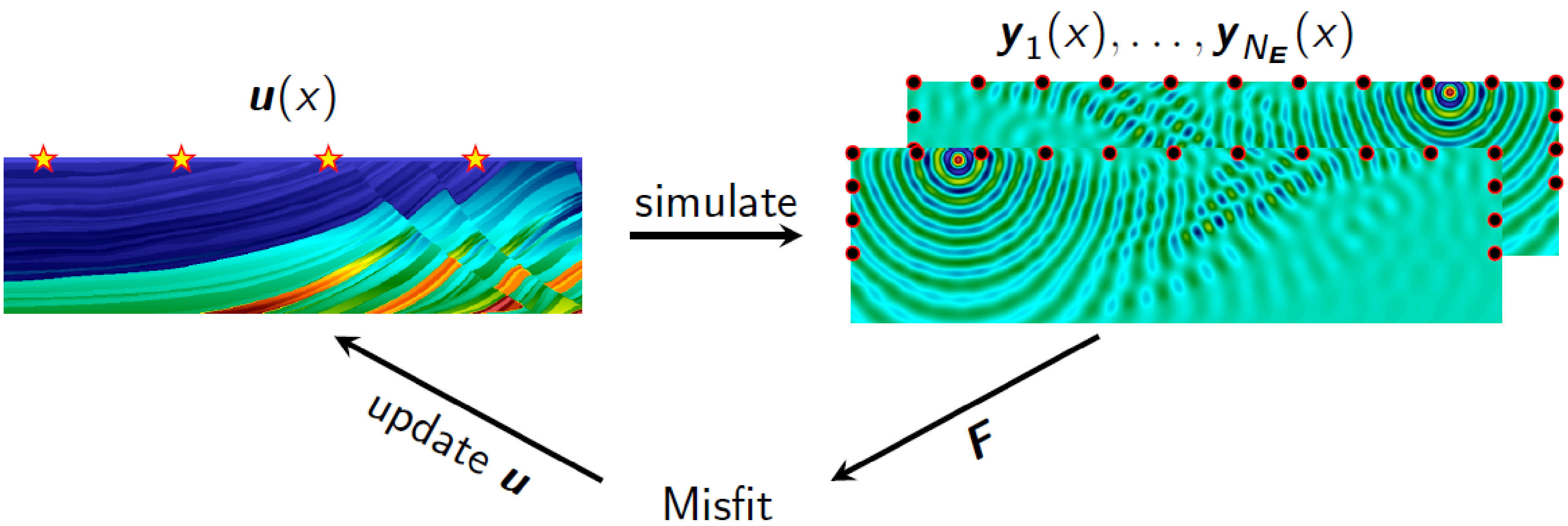
- Plug in parameters
  - Temporal frequency ω
  - Wave source f
  - Wave speed $u(x)$
- Simulate (discretize and solve) $\longrightarrow y(x)$



$u(x)$ $y(x)$

Application 3D Seismic imaging (ETH, USI)

- Given multiple sources ☆
- Measurements at location •
- Objective function $\boldsymbol{F}(\boldsymbol{y}, \boldsymbol{u})$ measures misfit of simulation and measurements
- Find $\boldsymbol{u}$ with best match of simulation an measurements: $\boldsymbol{F} \rightarrow min$



Application 3D Seismic imaging (ETH, USI)

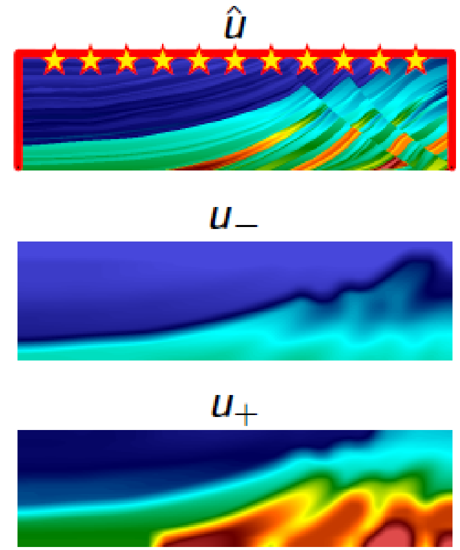
$$\min_{y,u} F(y,u) = \frac{1}{2}\sum_{k=1}^{N_E} \|v(y_k) - \hat{y}_k\|_{\ell^2}^2 + \frac{\alpha}{2} TV(u),$$

$$\text{s.t.} \; -\nabla \cdot (u^2 \nabla y_k) - \omega^2 y_k = \delta_k \qquad \text{in } \Omega,$$

$$\frac{\partial y_k}{\partial n} = i\frac{\omega}{u} y_k \quad \text{on } \partial\Omega,$$

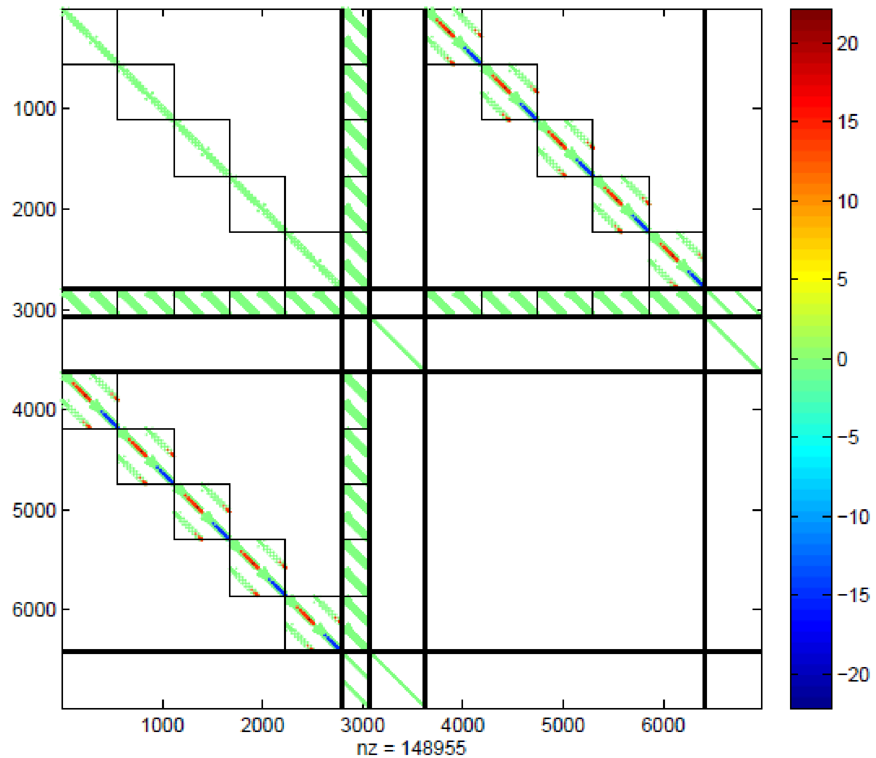
$$u_- \le u \le u_+.$$

- Simulate with $\hat{u}(x)$, Measure at 367 measurement points on $\partial\Omega$, add 1% noise
- Optimize using $N_E = 8,192$ sources
- Reconstruction with $N_E = 8,192$ PDEs



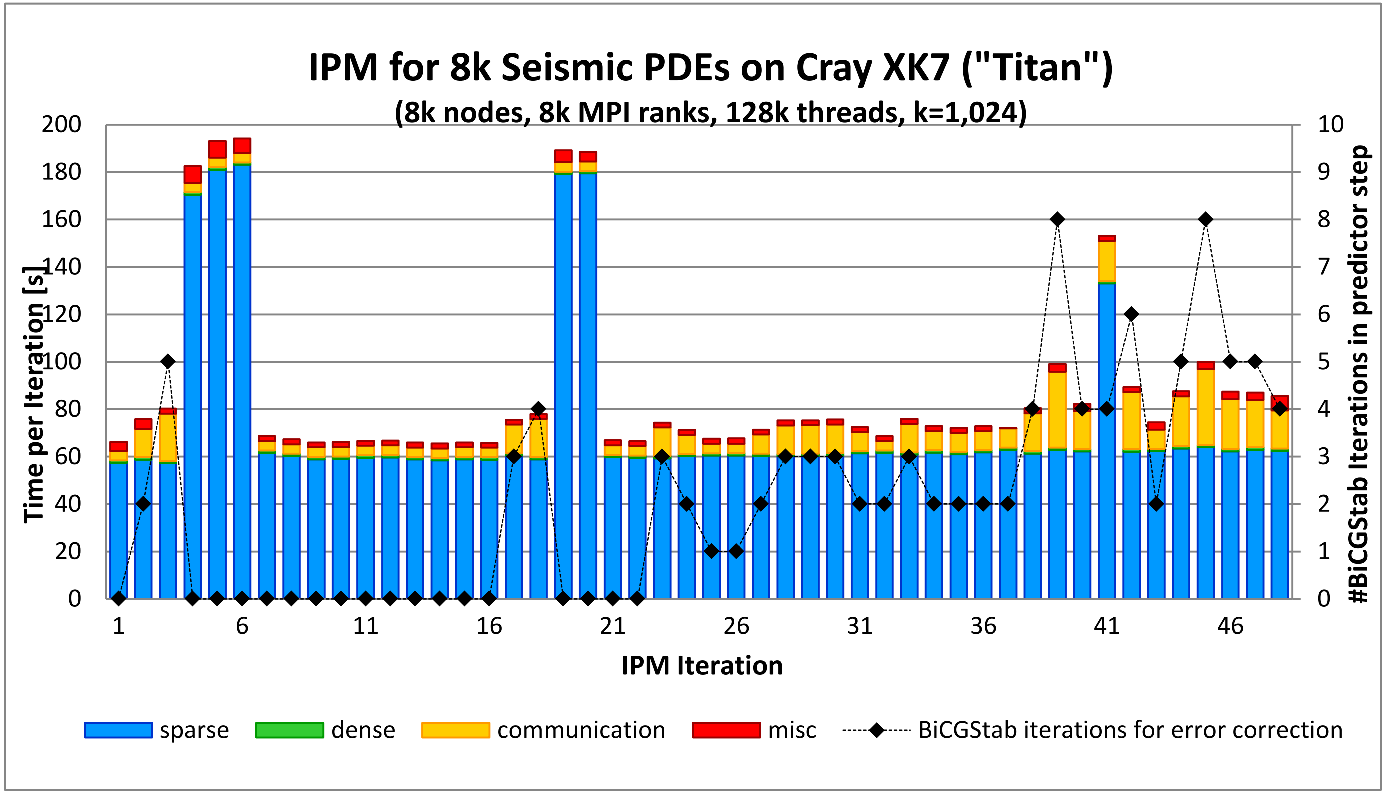
PDE-Constrained optimization, 5 PDEs, Arrow-shaped

- PDE-constrained optimization problem in 2D with five constraining complex-valued PDEs (Helmholtz).



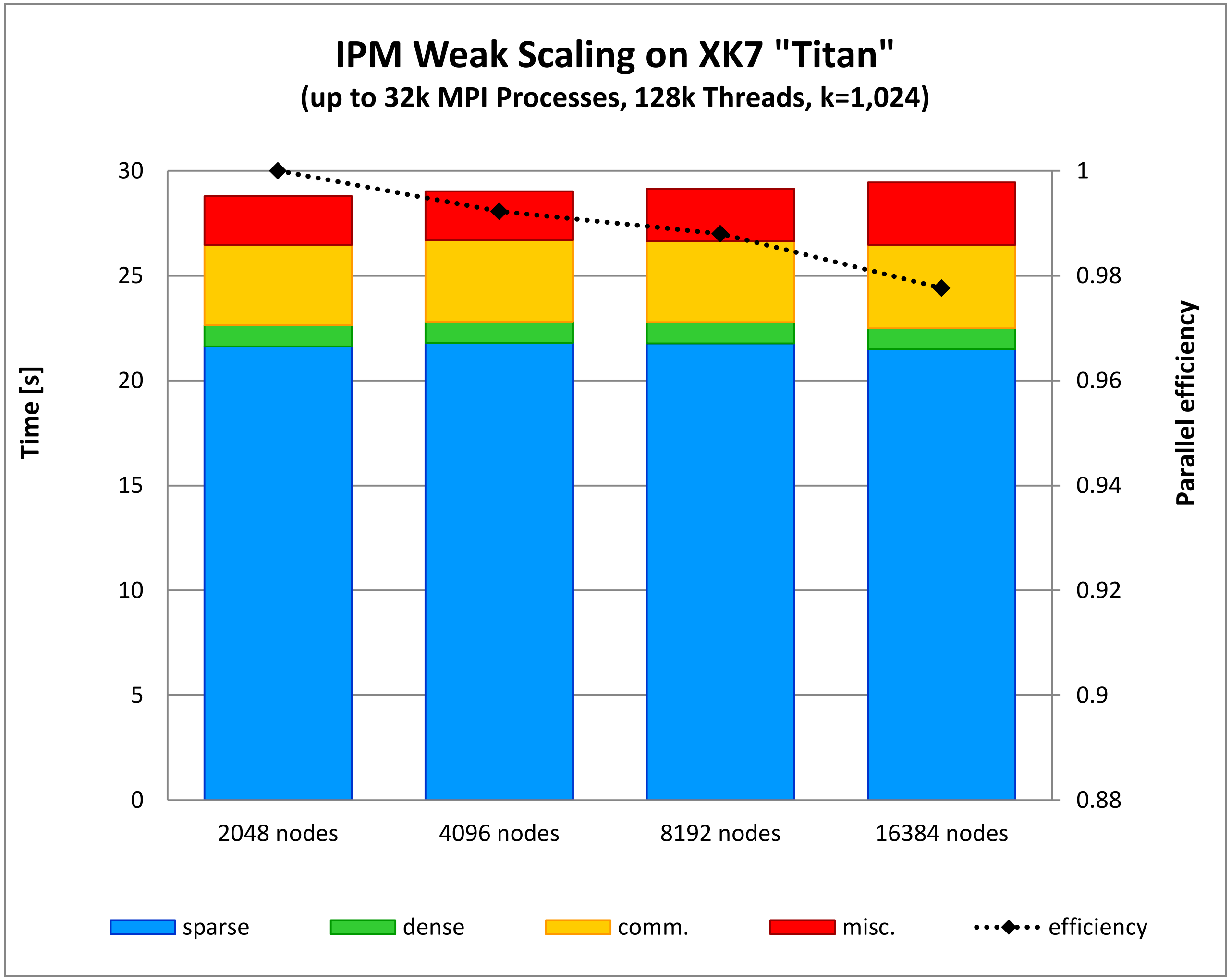
Time per IPM iteration up to 131,072 cores of "Titan"

- 3D seismic imaging problem (200^3), 8'192 Sensors ("Seismograms")
- 10,000s of control material variables -> NLP with several billions variables.

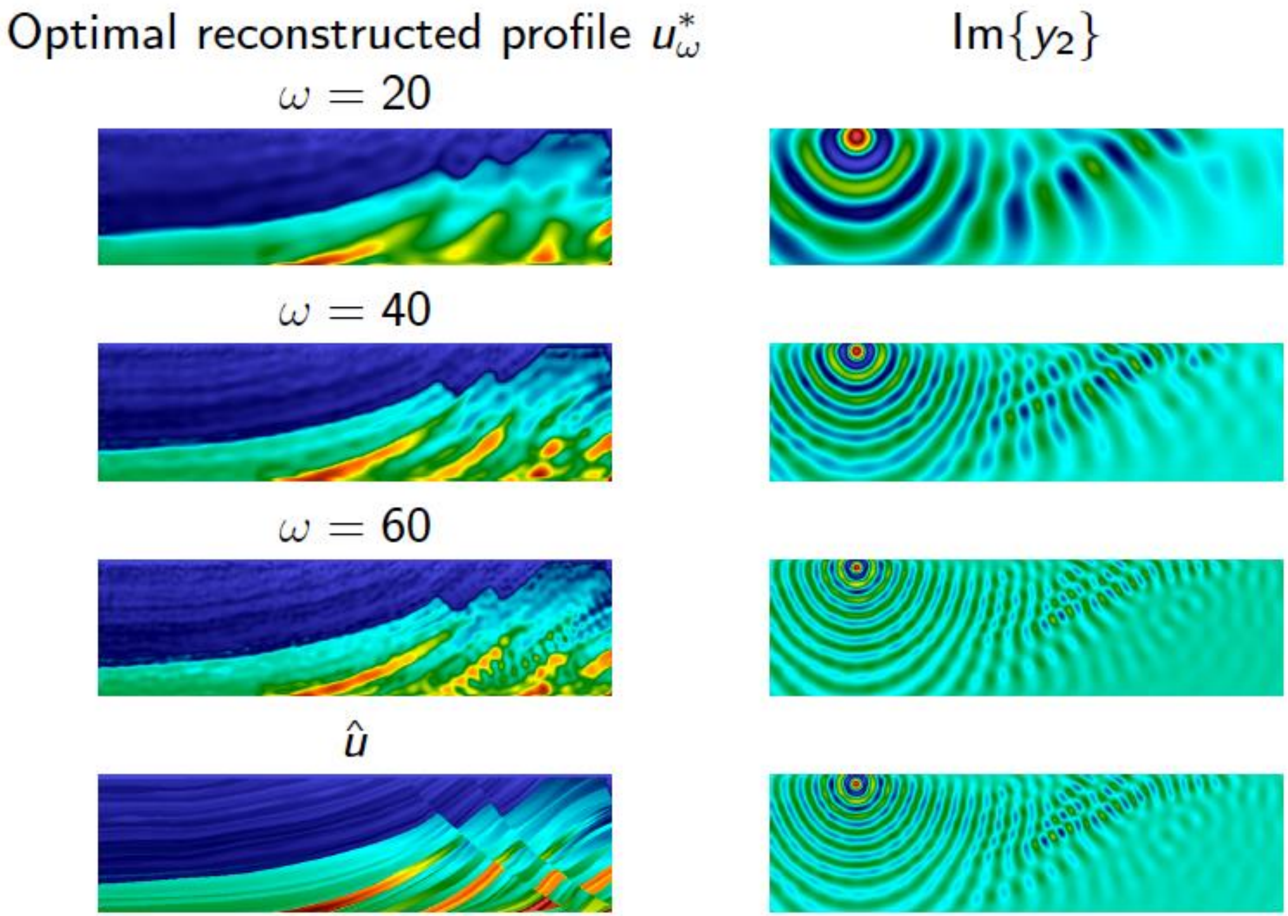


- Breakdown of the execution time for each IPM iteration when solving a seismic PDE-constrained optimization problem (Helmholtz) on 8'192 nodes.

IPM Weak Scaling in XK7 («Titan»)



Application 2D Seismic imaging (ETH, USI)



Conclusion

- Supercomputing: Re-design/Co-design algorithms to increase arithmetic intensity on manycores.
- Towards scalable algorithms and software for (semi-)structured nonlinear optimization problems (up to 262,114 cores on Titan).
- IPM can converge in a small number of iterations for very large-scale problems.
- Application in Switzerland: 3D Seismic imaging.

- Application: First real-time stochastic optimization in power grid applications (Argonne)
  - C. Petra, O. Schenk, M.Lubin, K. Gärtner, An augmented incomplete factorization approach for computing the Schur complement in stochastic optimization, SIAM J. Sci. Comput, in press.
  - C. G. Petra, O. Schenk, M. Anitescu, *Real-time Stochastic Optimization of Complex Energy Systems on High Performance Computers.* Submitted to IEEE CiSE.

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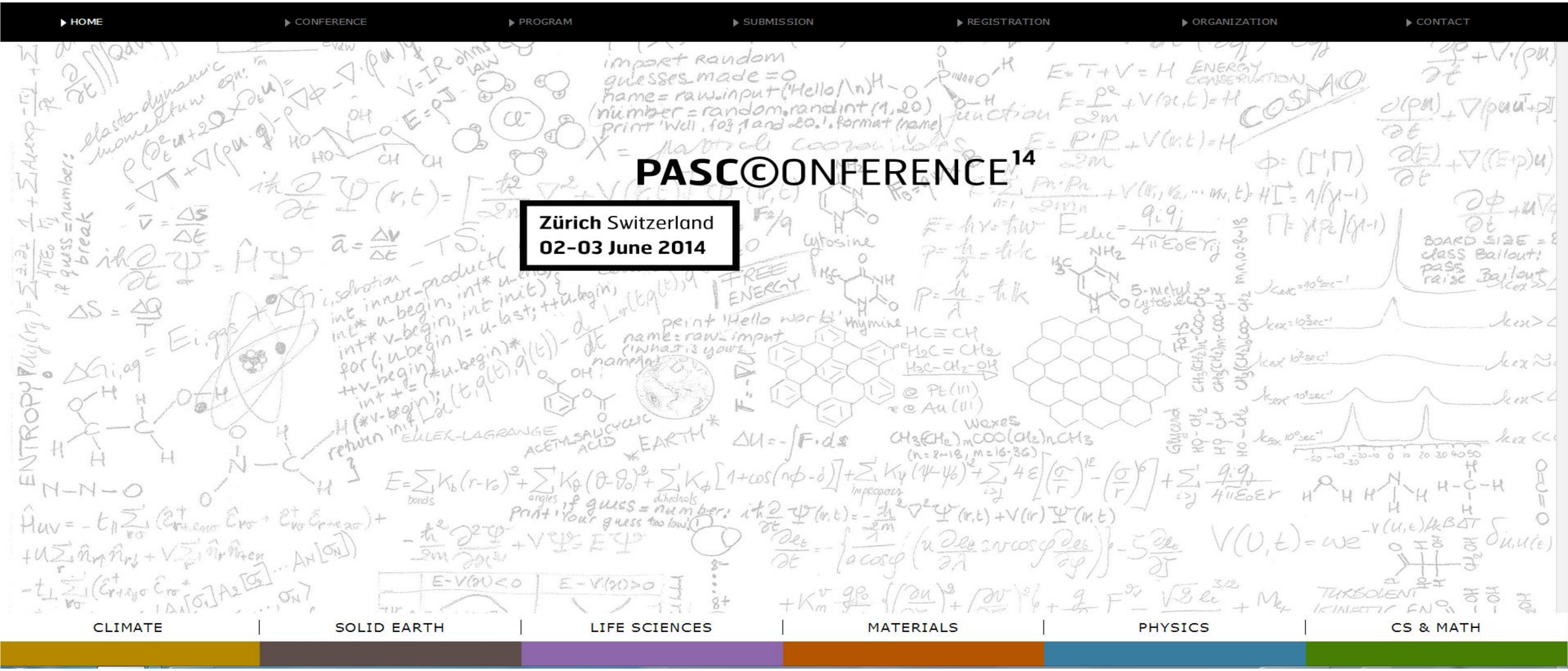

- **www.pasc14.org, 7 invited plenary talk, 60 contributed talks + poster session**
- **Abstract deadline: March 31, 2014.**

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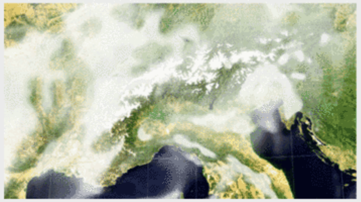
Climate Network



INVITED TALKS

Weather and Climate modelling at the Petascale: achievements and perspectives

Pier Luigi Vidale, University of Reading, United Kingdom

Increasing availability of high-performance computing has allowed the climate modeling community to construct a new generation of global coupled models, capable of resolving some of the fundamental processes that govern the climate system. More explicit representation of eddies in the ocean and of weather systems in the atmosphere has demonstrated how they contribute to the general circulation and how it is increasingly possible to rely less on uncertain physical parameterisations. These developments are potentially promising for reducing inter-model disagreement in community multi-model hindcasts and projections. We have demonstrated, for instance, how the representation of the relative importance of the remote and local processes governing the global energy and hydrological cycles converges at resolutions beyond 50km. These so-called "weather-resolving" climate models are also suitable for studying how global teleconnections might influence the long-term regional changes in storm tracks, or in understanding changes in high-impact phenomena, such as Tropical and Extra-Tropical Cyclones, as well as their contributions to the general circulation.

Some of the leading Global Climate Models have already started to operate in the so-called "grey zone", removing some long-standing errors in the simulation of the diurnal cycle of precipitation, as well as improving the intensity/frequency relationship. However, major uncertainties remain with respect to the adequateness of key parameterizations, such as turbulence and microphysics, when operating over these interim scales, an open problem until true global cloud-resolving capability can be developed.

Pier Luigi Vidale is full professor at the University of Reading and a senior scientist at the National Centre for Atmospheric Science (NCAS-Climate), leading and developing research on High-Resolution Global Climate Modelling and biosphere-atmosphere interactions.

- www.pasc14.org, 7 invited plenary talk, 60 contributed talks + poster session
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- Markus Püschel, ETH Zurich
- Olaf Schenk, Università della Svizzera italiana

INVITED TALK

Engineering for Performance in High Performance Computing

Bill Gropp, Director of the Parallel Computing Institute, University of Illinois Urbana-Champaign

Achieving good performance on any system requires balancing many competing factors. More than just minimizing communication (or floating point or memory motion), for high end systems the goal is to achieve the lowest cost solution. And while cost is typically considered in terms of time to solution, other metrics, including total energy consumed, are likely to be important in the future.

Making effective use of the next generations of extreme scale systems requires rethinking the algorithms, the programming models, and the development process. This talk will discuss these challenges and argue that performance modeling, combined with a more dynamic and adaptive style of programming, will be necessary for extreme scale systems.

Bill Gropp is Thomas M. Siebel Chair in Computer Science since 2013. Gropp is a Fellow of ACM, IEEE, and SIAM, and a member of the National Academy of Engineering. He received the Sidney Fernbach Award from the IEEE Computer Society in 2008 and the TCSC Award for Excellence in Scalable Computing in 2010.

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Thanks for your attention.