Towards Exascale: The growing pains of Industry-strength engineering software

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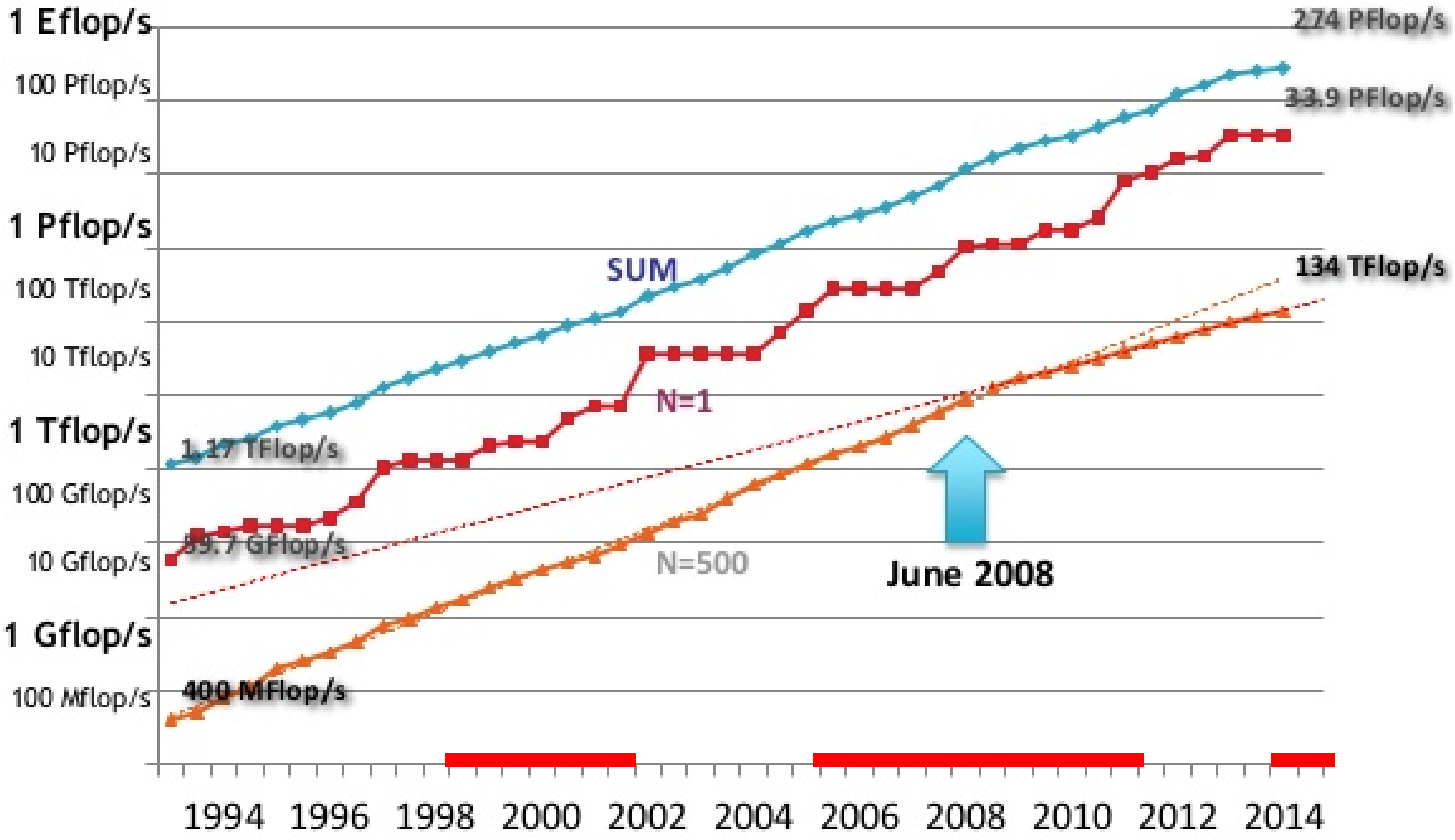
KEEP
CALM
AND
FOCUS ON
OPEN SOURCE

Hardware

Performance Development

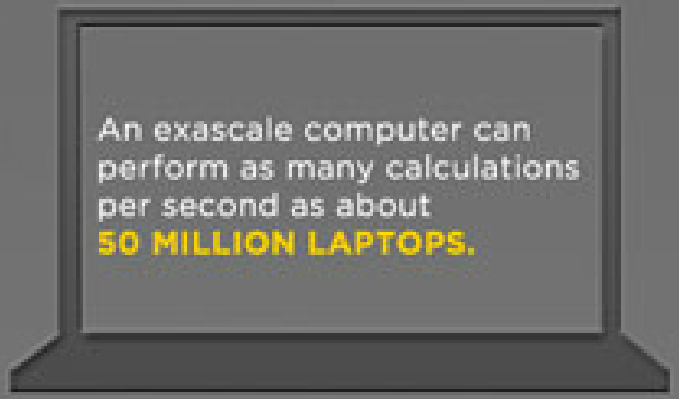


299,008 cores (Opteron) and 18,600 NVIDIA GPUs
>20,000,000,000,000,000 floating point operations per second

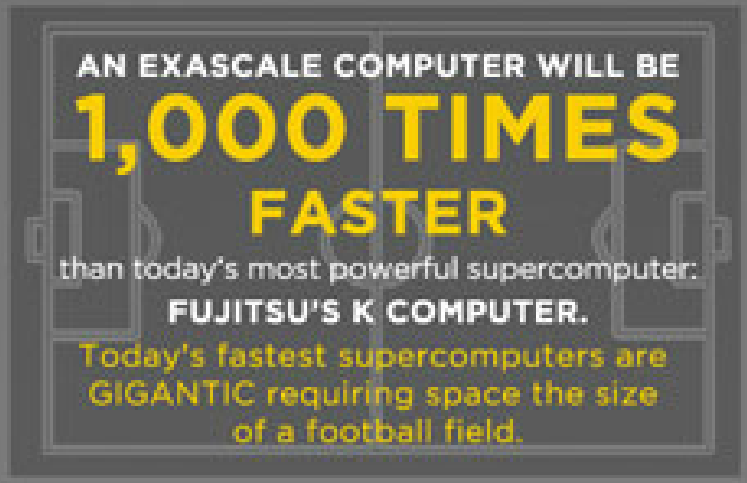
3,120,000 cores (Intel Ivy Bridge and Xeon Phi)
33,860,000,000,000,000 floating point operations per second

1,000,000,000,000,000,000

AN **EXASCALE** COMPUTER WILL PERFORM **ONE QUINTILLION** OPERATIONS **PER SECOND.**



Current projections for power consumption of exascale computers is put at **100 MEGAWATTS** – the same amount of power as **ONE MILLION 100-WATT** lightbulbs.



2018?

Scientists hope to build an exascale computer by 2018 with the **Europe, China, Japan and the U.S.** all investing hundreds of millions of **$$$**.

The processing power will transform sciences such as **astrophysics and biology** as well as improving **climate modelling and national security**.


Evolution
of
Tomb Raider
http://larreks.deviantart.com/art/Evolution-of-Tomb-Raider-425582963
Larreks

#1 in 1996?

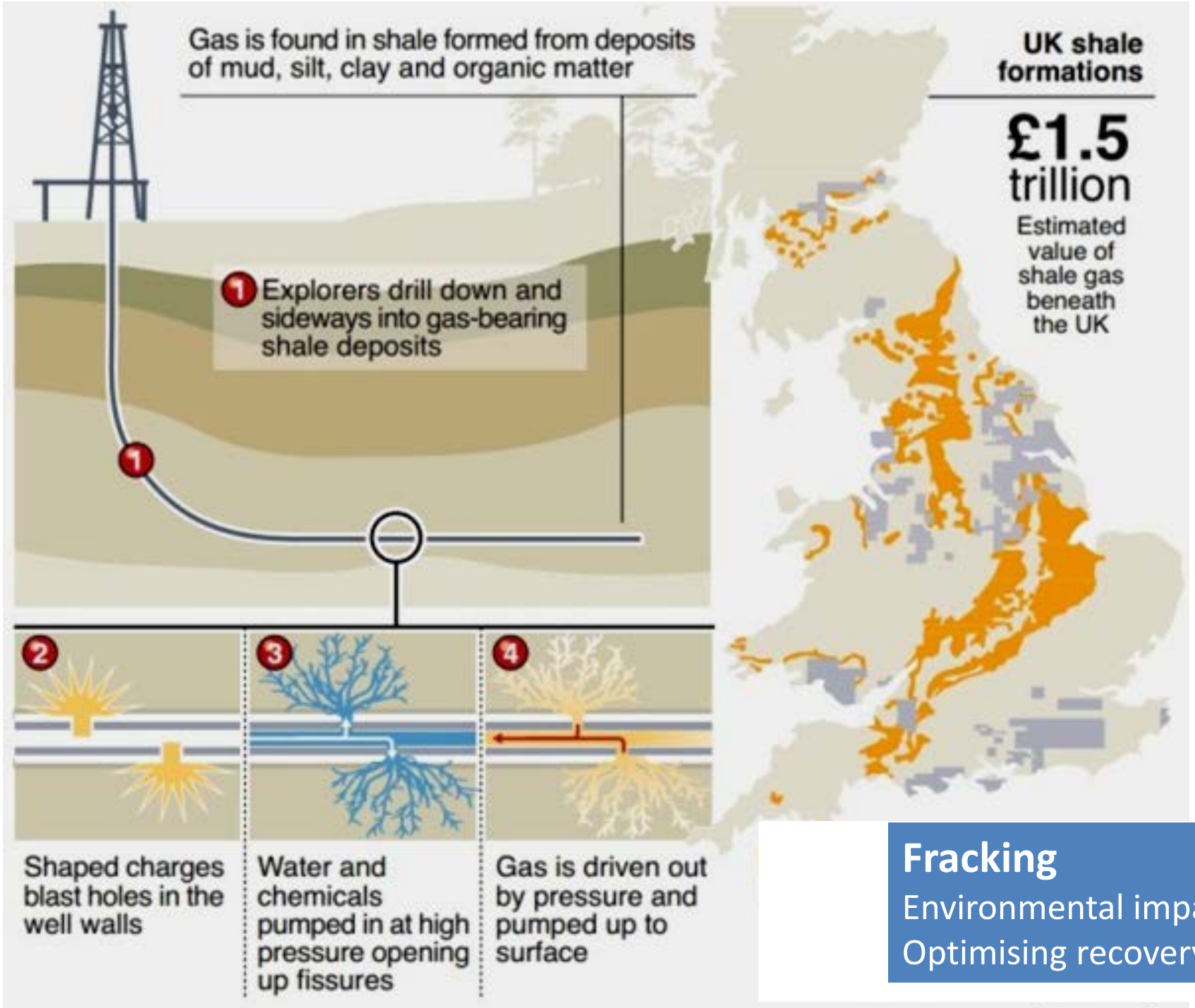
A8 Processor SoC
~172GFlops?

Exascale Workstation in 2030?

Source: engineering.com

Challenging Engineering

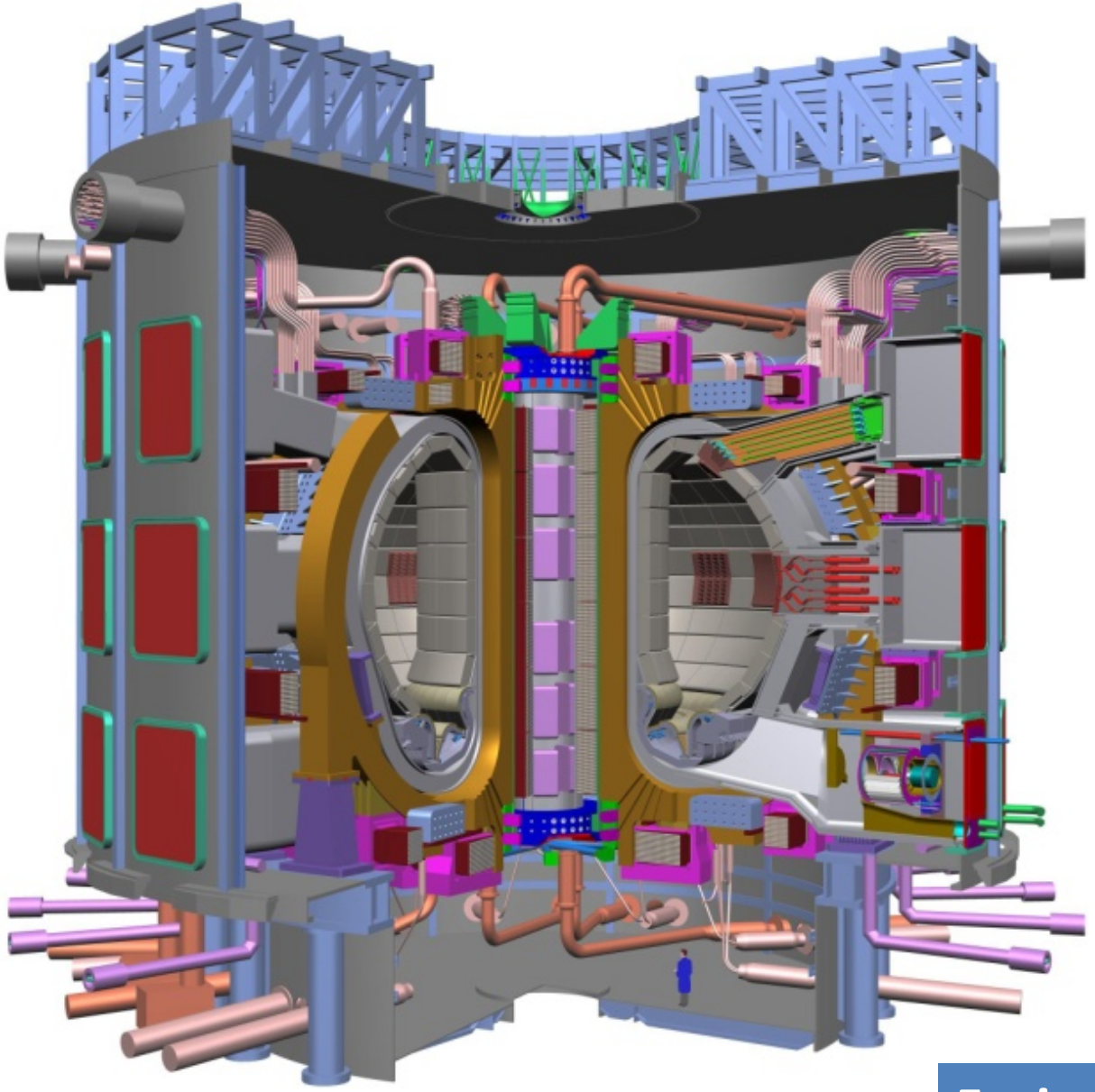
Wind farm modelling
Noise, efficiency
Structural integrity
Environmental impact



Fracking

Environmental impact

Optimising recovery



ITER: Estimated construction cost for physical prototype is around 13 Billion €

Fusion Energy
Design new materials
Virtual prototypes?

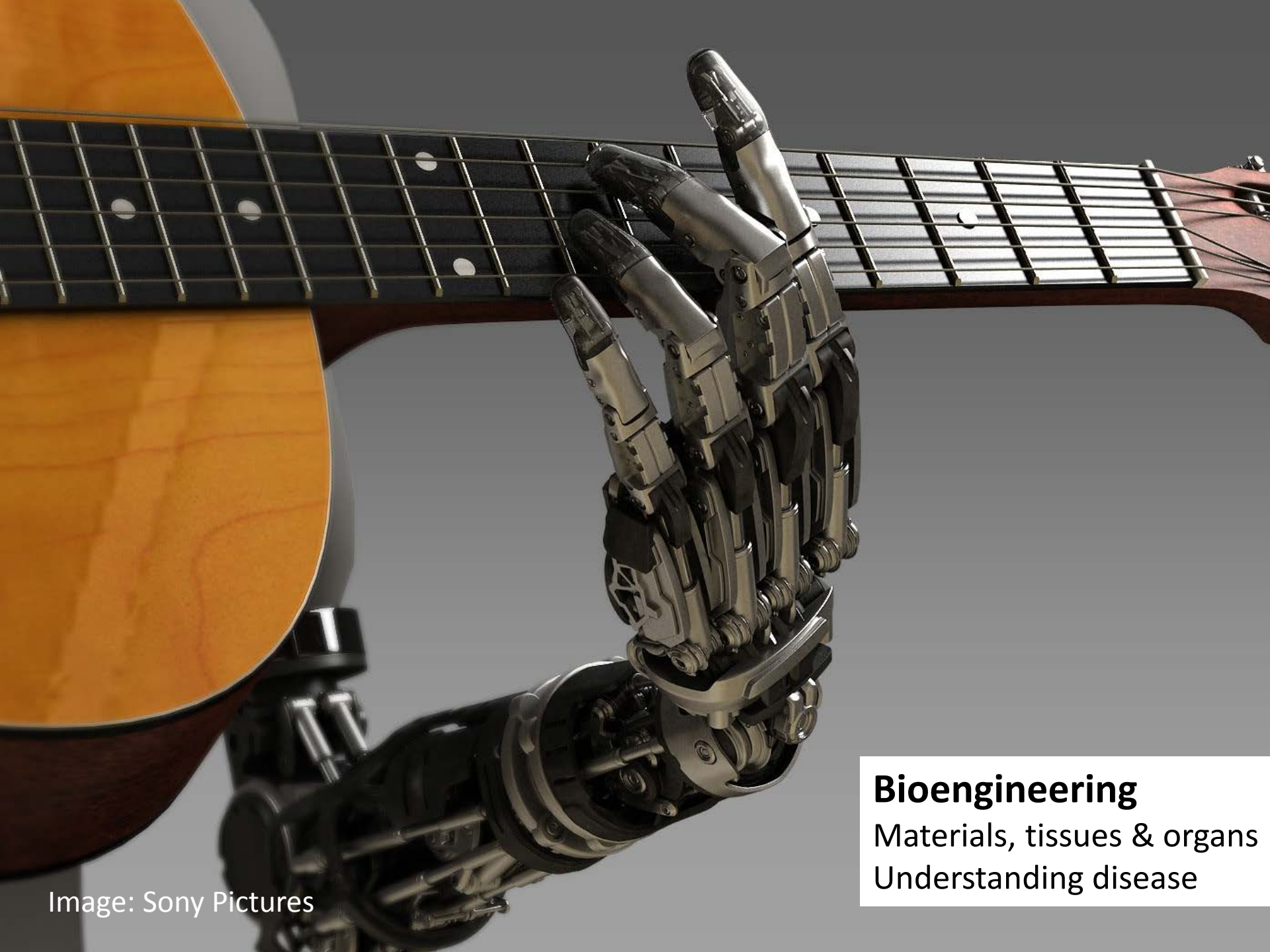
Massive Takata Airbag Recall: Everything You Need to Know, Including Full List of Affected Vehicles

Transport

Ageing of materials

Manufacturing defects

Systems vs components



Bioengineering

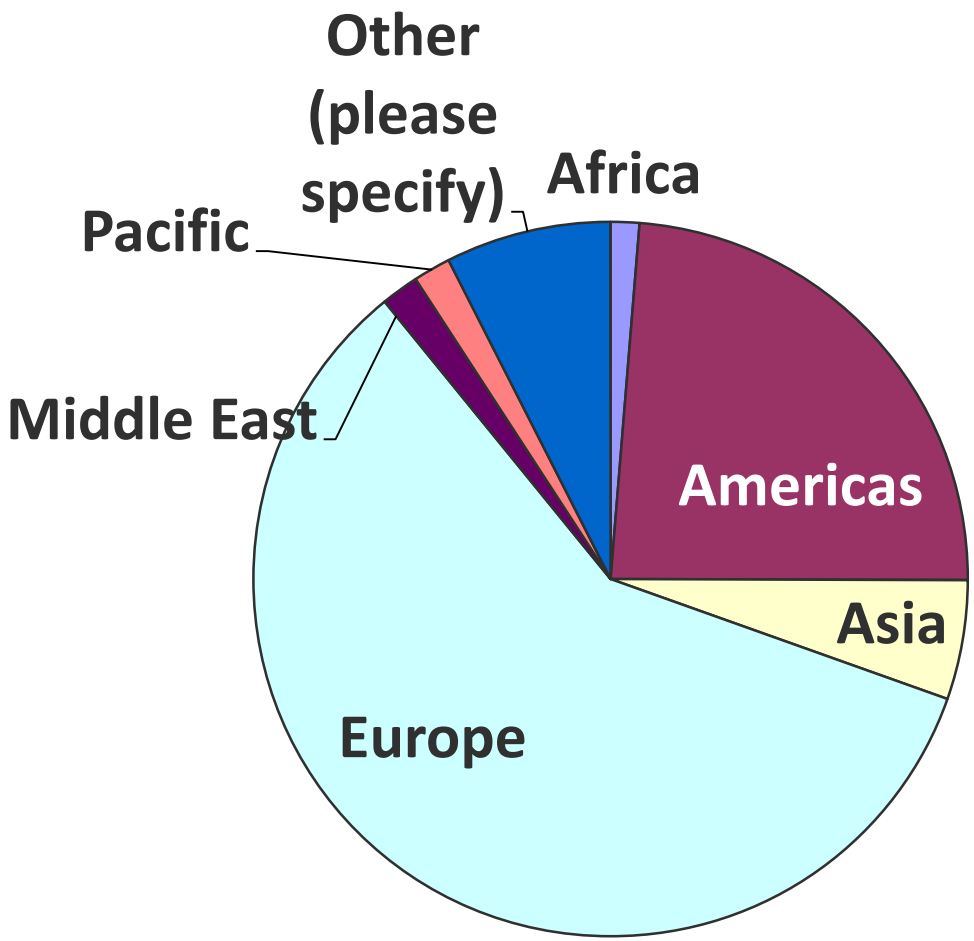
Materials, tissues & organs

Understanding disease

Image: Sony Pictures

Engineering Simulation in Industry Today

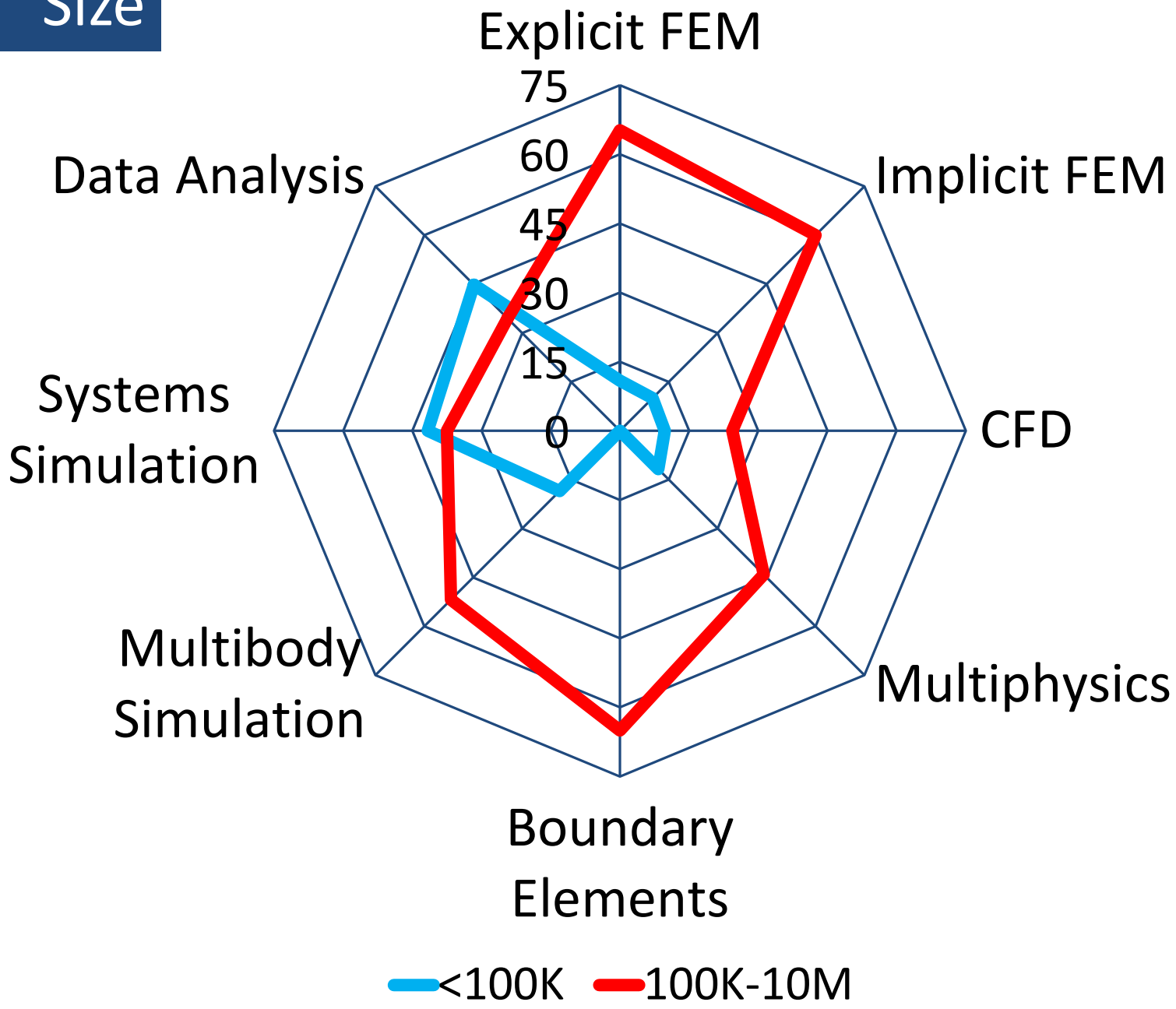
Computing Platforms for Engineering Simulation

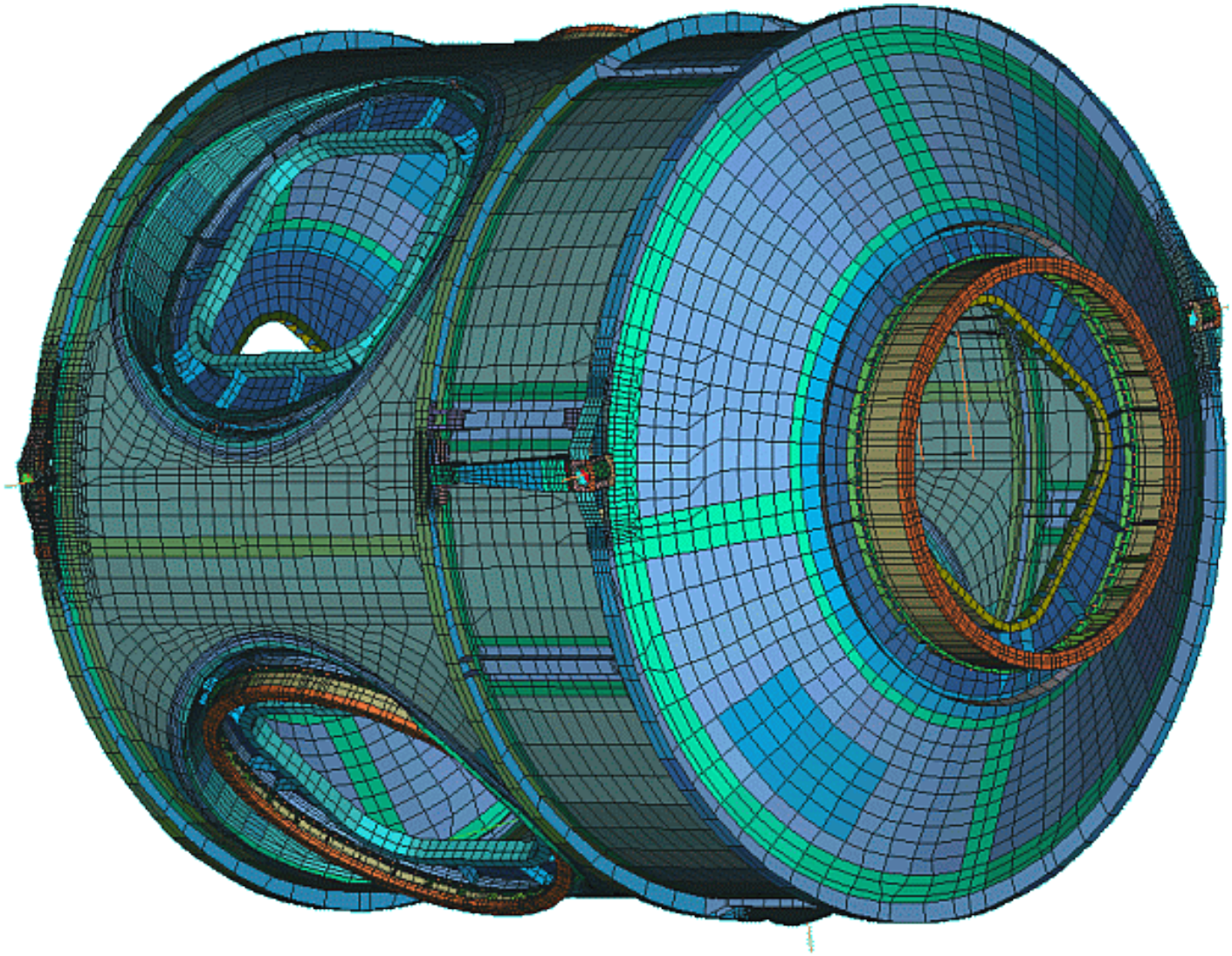


Sep to Nov 2014
Around 250 Respondents
Questions directed at firms

http://www.nafems.org
http://www.eesi-project.eu/

Size

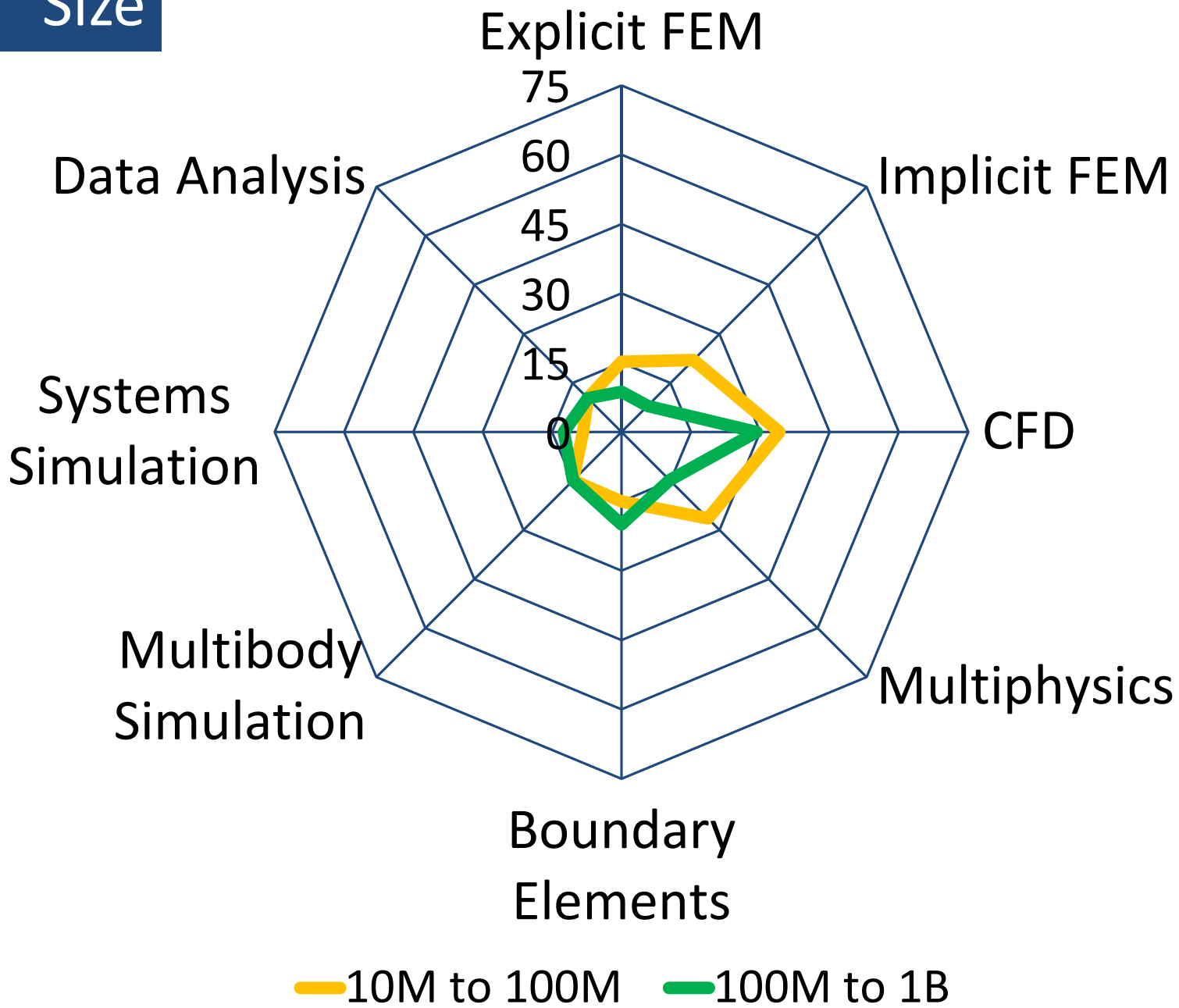

Explicit FEM
75
60
45
30
15
0
Implicit FEM
CFD
Multiphysics
Boundary Elements
Multibody Simulation
Systems Simulation
Data Analysis
<100K
100K-10M

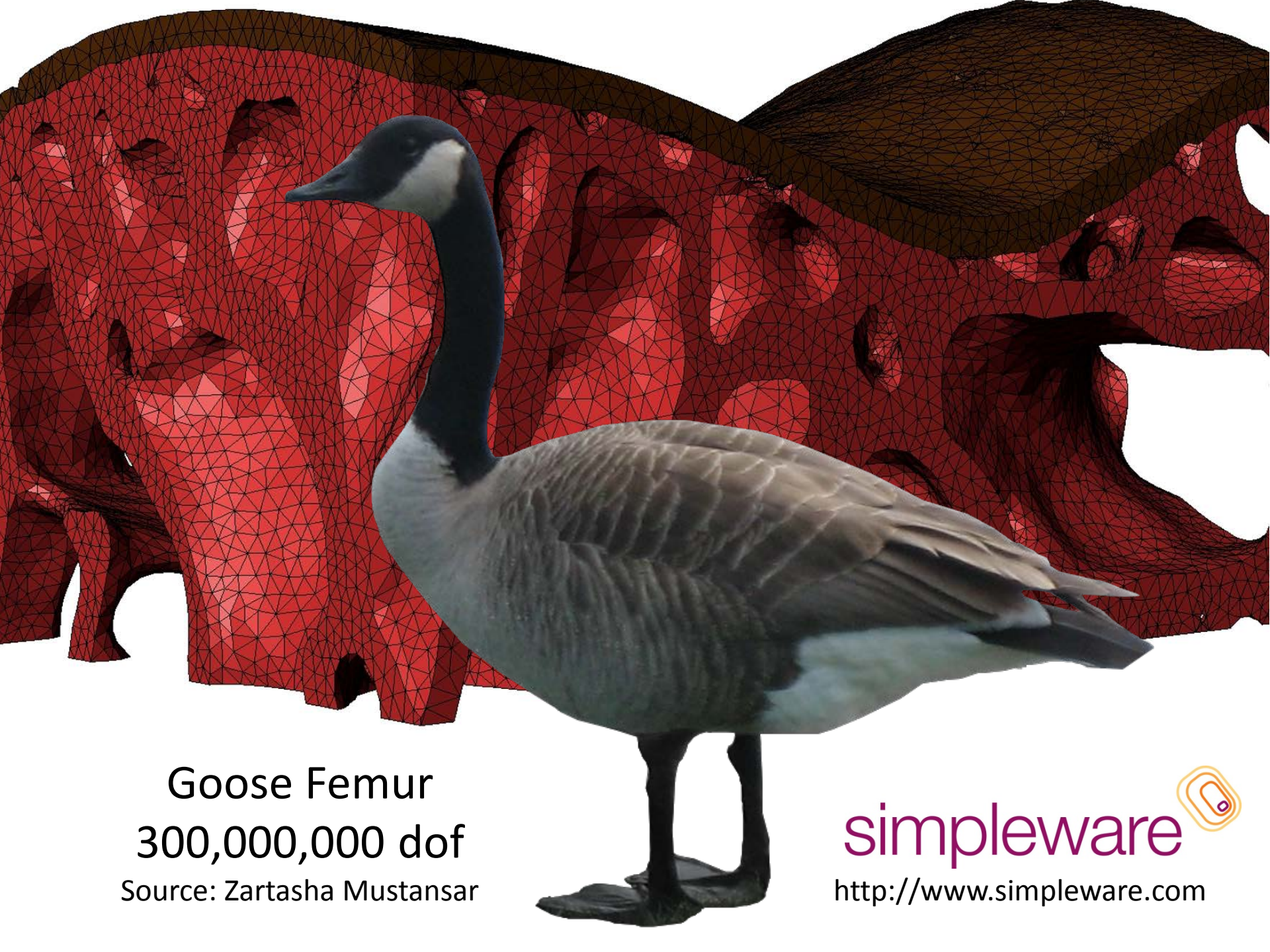


International Space Station Component
250,000 degrees of freedom (dof) circa 1999

Source: http://www.tobynorris.com

Size

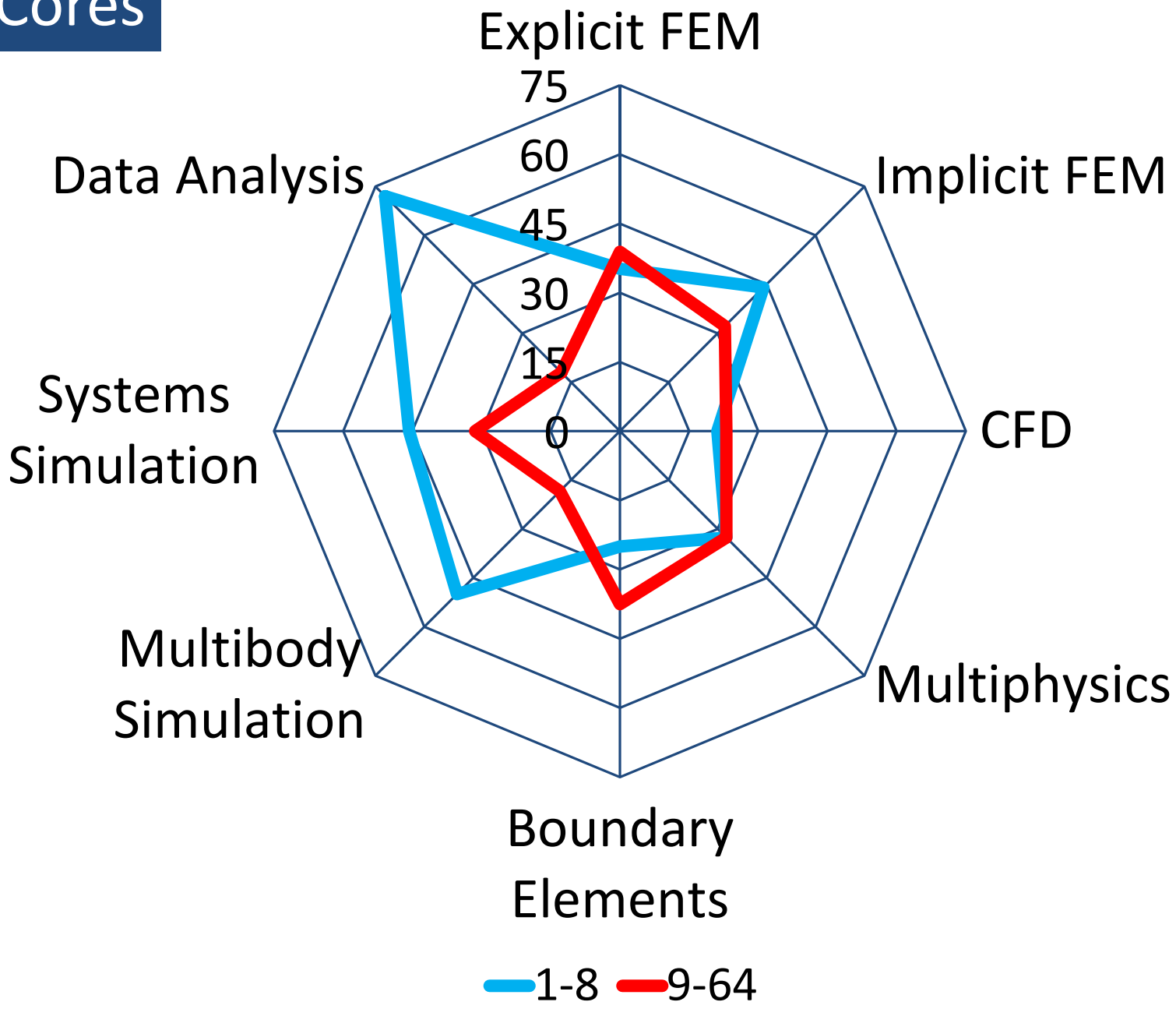

Explicit FEM
75
60
45
30
15
0
Implicit FEM
CFD
Multiphysics
Boundary Elements
Multibody Simulation
Systems Simulation
Data Analysis
10M to 100M
100M to 1B



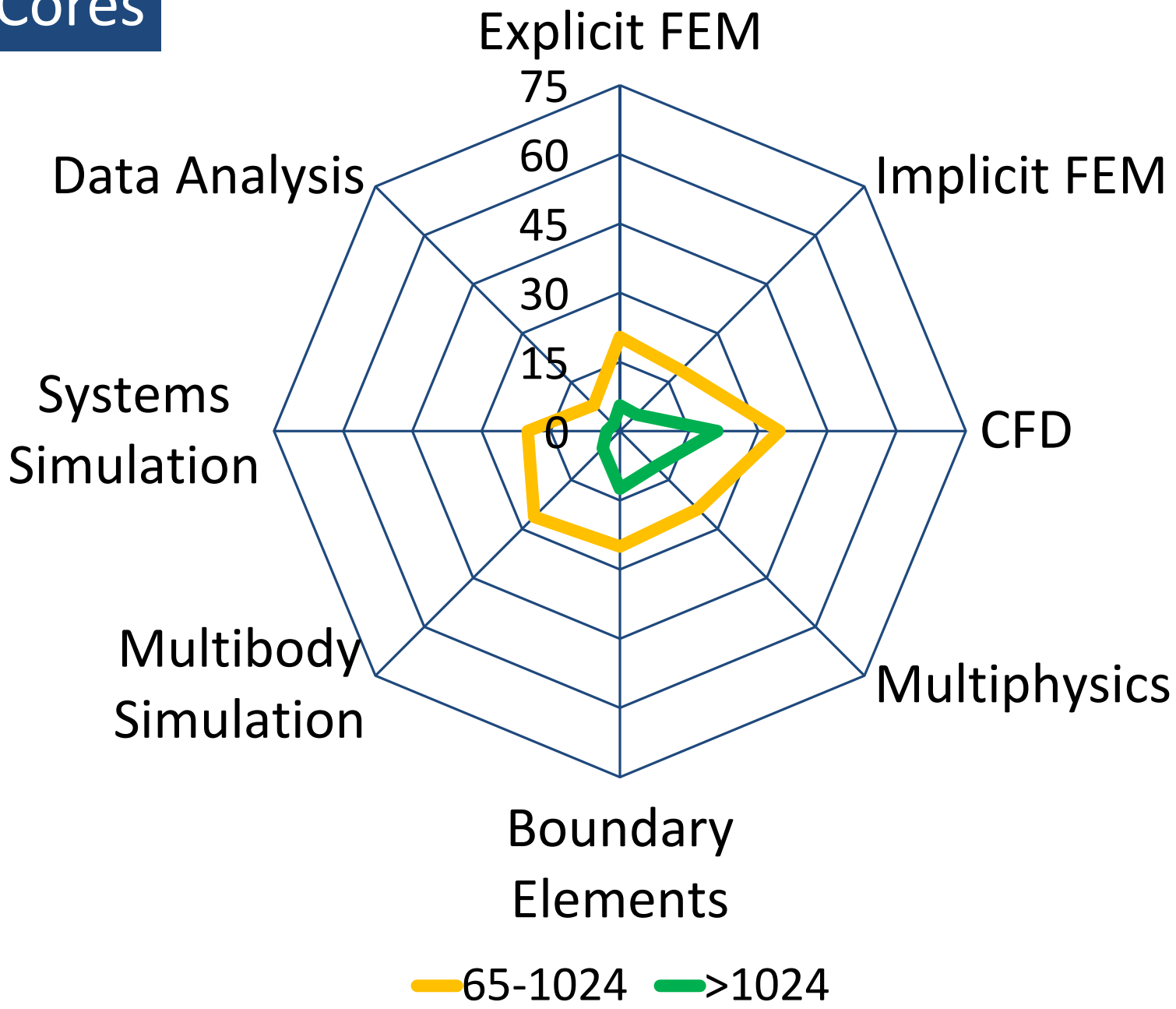
Goose Femur
300,000,000 dof
Source: Zartasha Mustansar

simpleware
http://www.simpleware.com

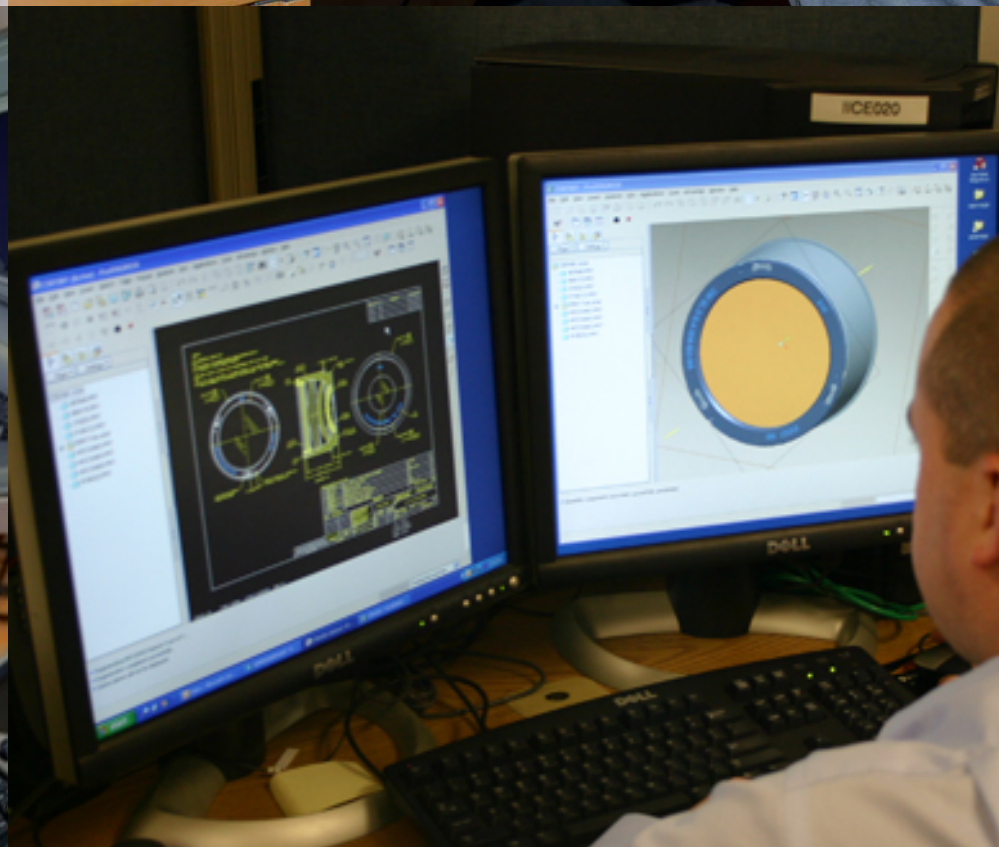
Cores

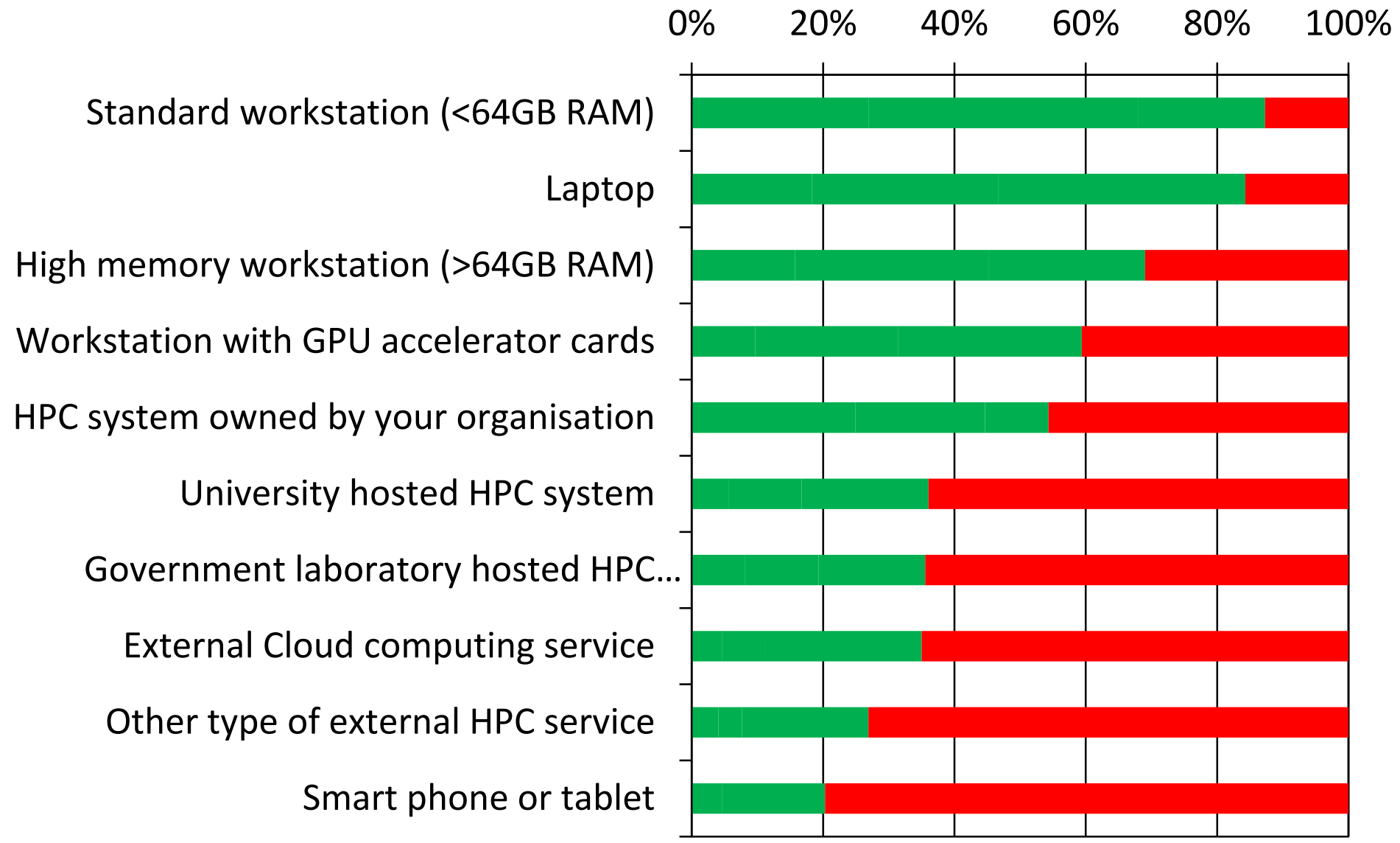

Explicit FEM
75
60
45
30
15
0
Implicit FEM
CFD
Multiphysics
Boundary Elements
Multibody Simulation
Systems Simulation
Data Analysis
1-8
9-64

Cores

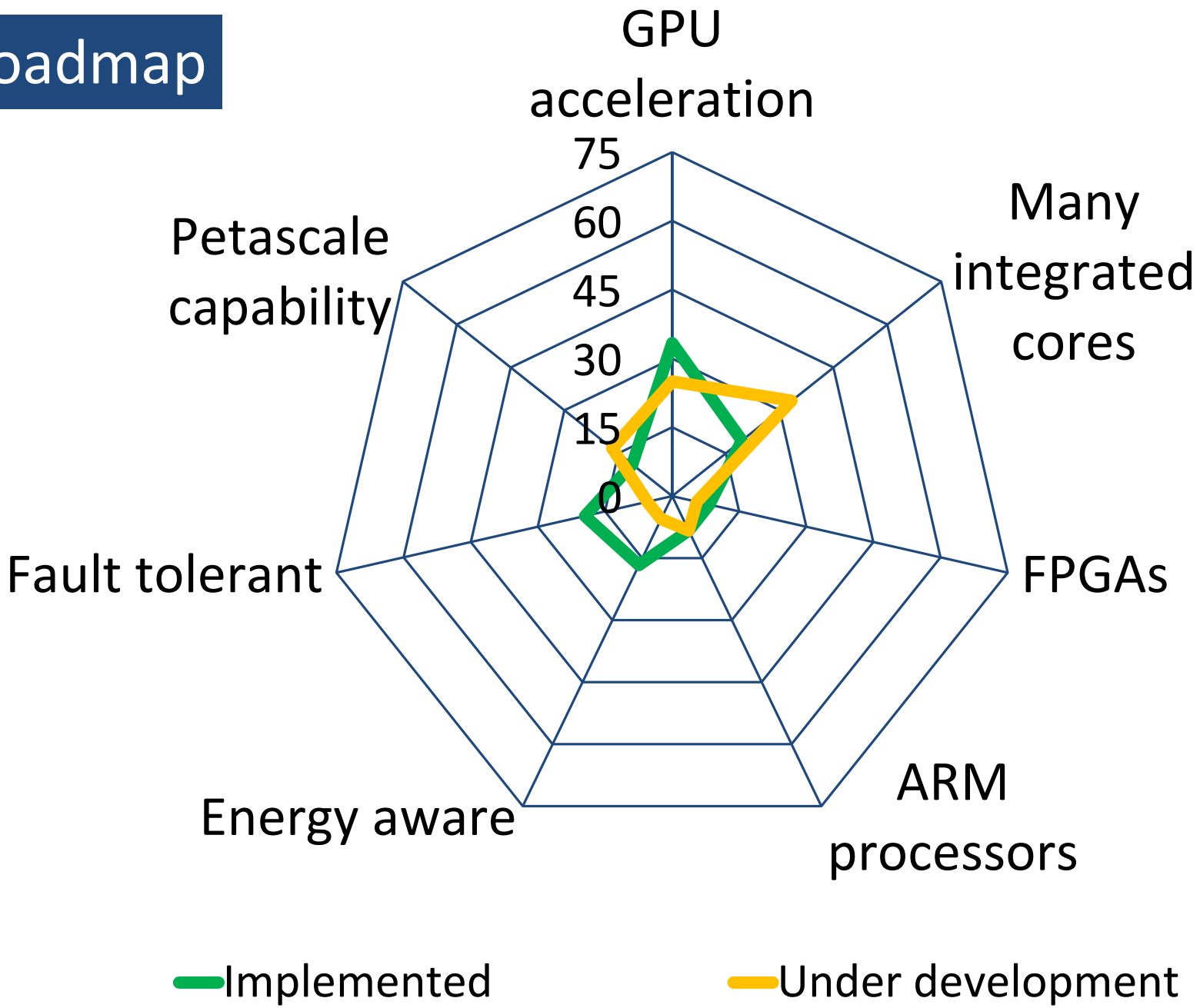

Explicit FEM
75
60
45
30
15
0
Implicit FEM
CFD
Multiphysics
Boundary Elements
Multibody Simulation
Systems Simulation
Data Analysis
65-1024
>1024


SAMSUNG

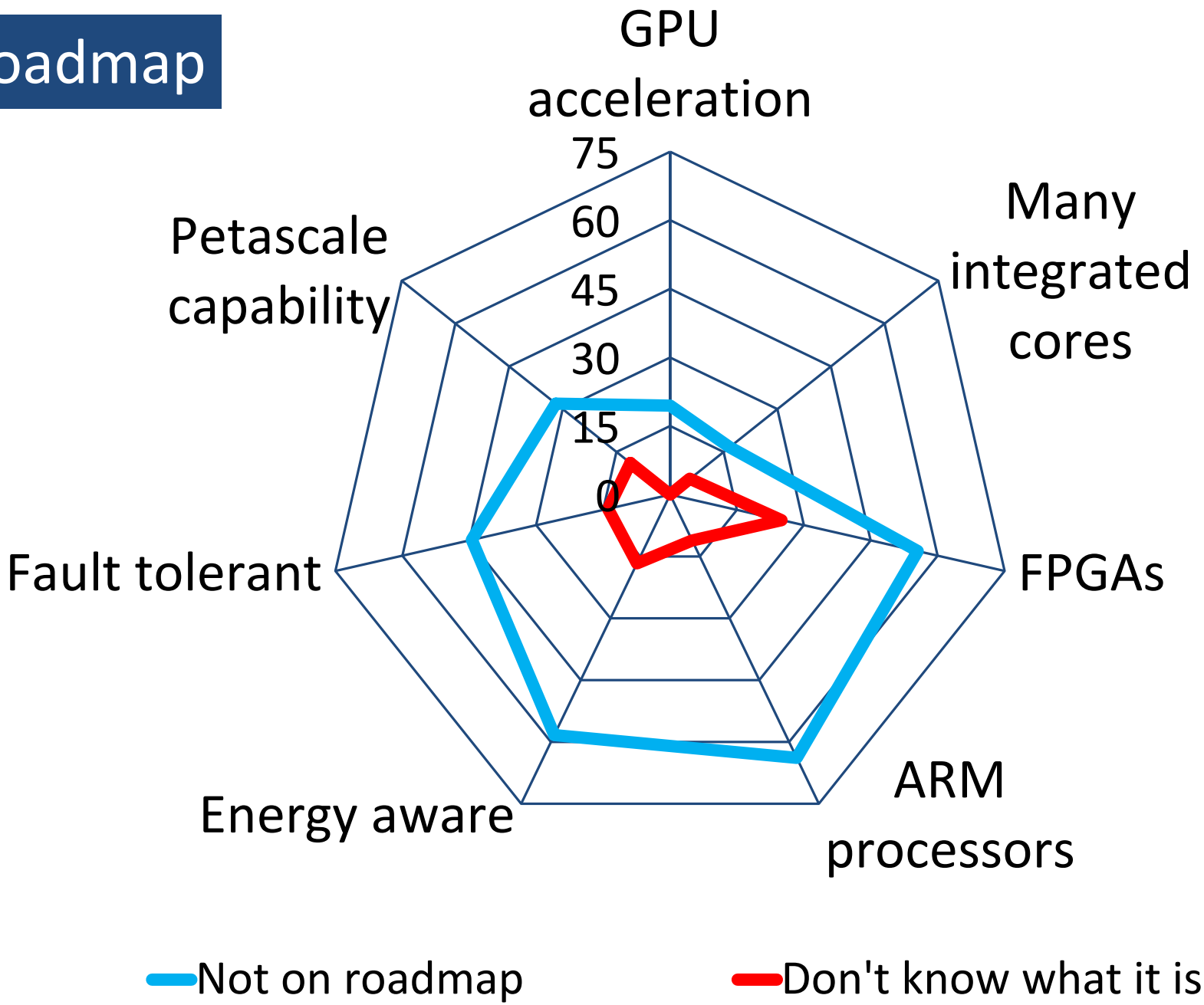

DELL


0%
20%
40%
60%
80%
100%
Standard workstation (<64GB RAM)
Laptop
High memory workstation (>64GB RAM)
Workstation with GPU accelerator cards
HPC system owned by your organisation
University hosted HPC system
Government laboratory hosted HPC…
External Cloud computing service
Other type of external HPC service
Smart phone or tablet

Roadmap


GPU acceleration
75
60
45
30
15
0
Many integrated cores
FPGAs
ARM processors
Energy aware
Fault tolerant
Petascale capability
Implemented
Under development

Roadmap


GPU acceleration
75
60
45
30
15
0
Many integrated cores
FPGAs
ARM processors
Energy aware
Fault tolerant
Petascale capability
Not on roadmap
Don't know what it is

Open Source Software

*“ … is provided under a software license that permits users to **study, change, improve** and at times also to distribute the software.”*

Wikipedia

*“ … The new leaders in innovation will be those who figure out the best way to **leverage a network of outsiders**.”*

Pisano and Verganti 2008

Participation

Motivation

Software use value
Status and recognition
Learning
Personal enjoyment
Reciprocity
Getting paid
Sense of ownership and control
Career advancement
Free software ideology
Helping others
Social identity

Demographic

Gender	98.9% Male
Average Age	27

Education

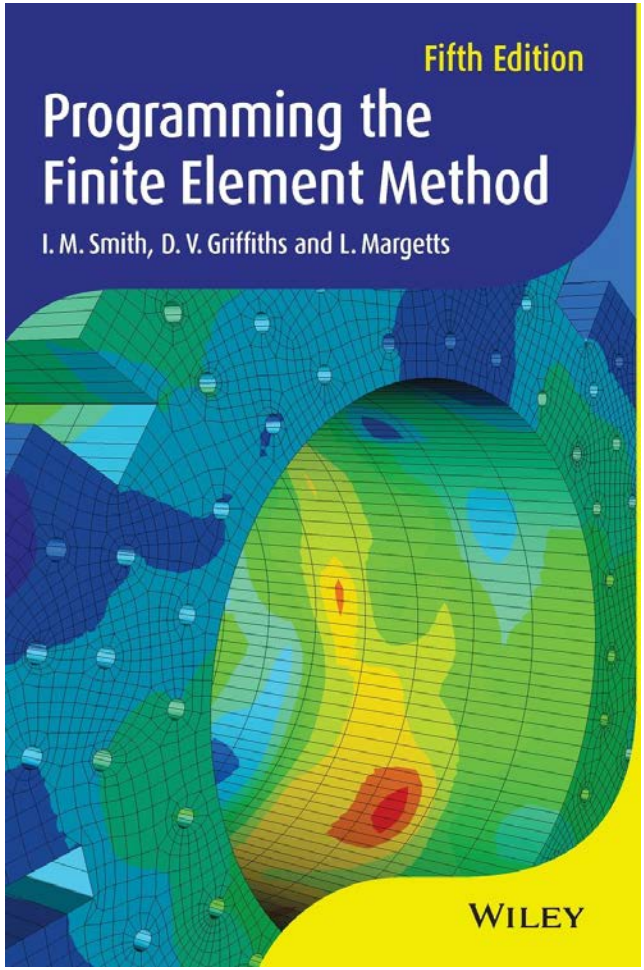
College	33%
Master	28%
PhD	9%

Employment

Students	20%
IT Jobs	58%

Source: Ghosh et al., 2002

ParaFEM –Parallel Finite Element Analysis

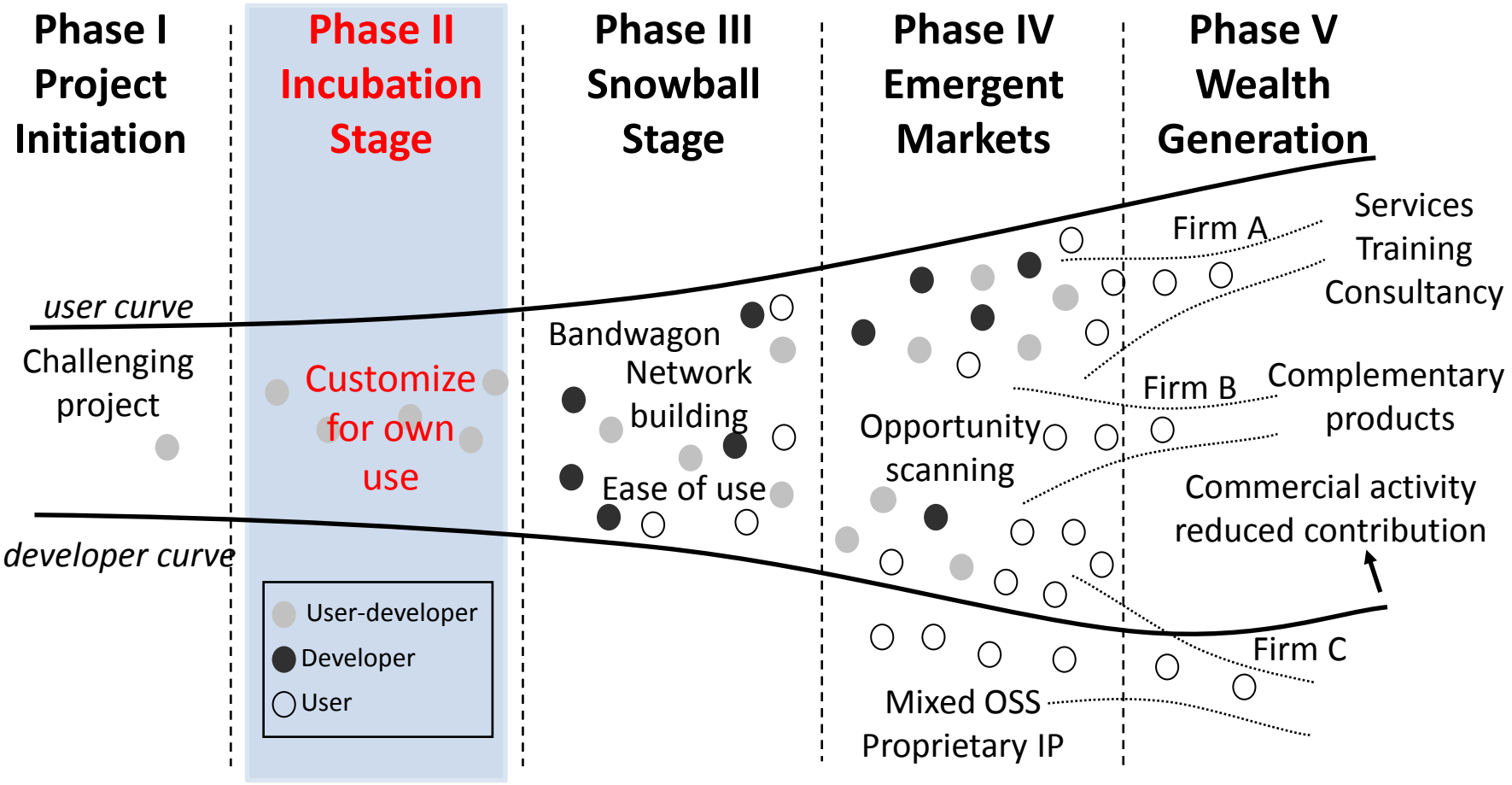


- Open source library + ~70 mini Apps
- ~64,000 cores
- >1 billion degrees of freedom
- Used for teaching and research
- 750+ registered on website
- ~1000 citations of text book

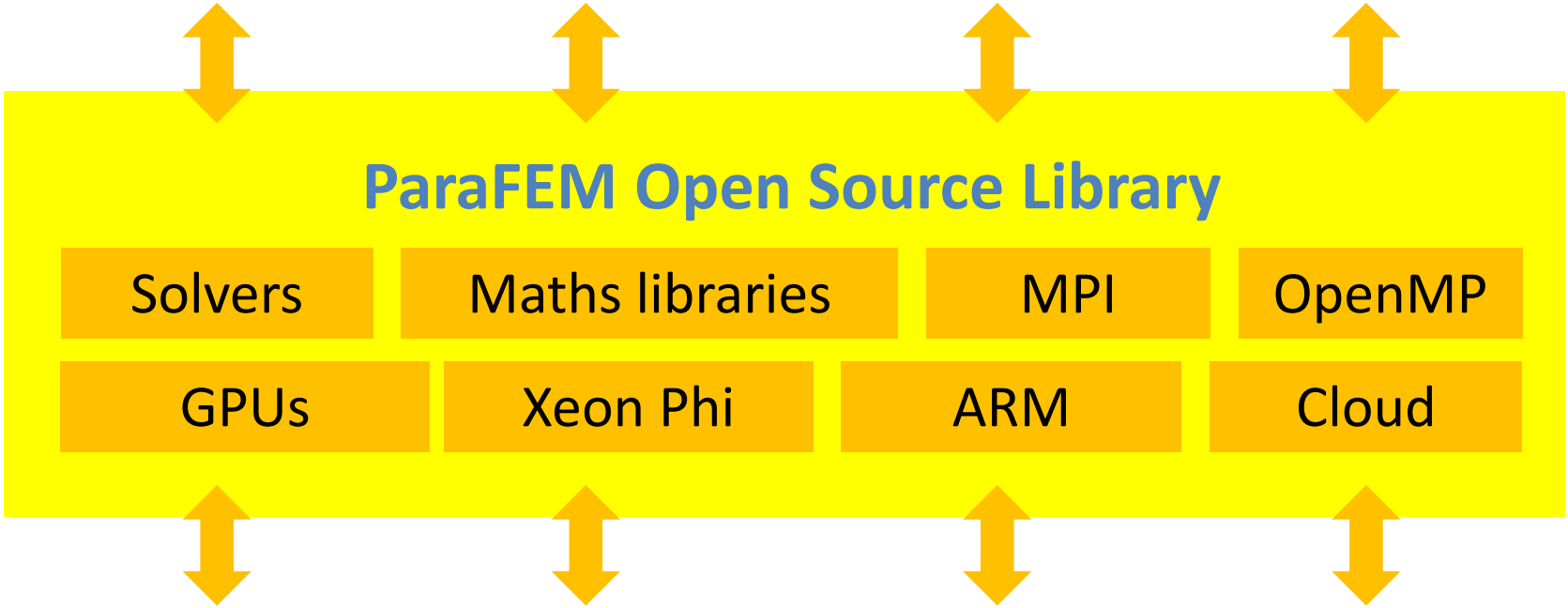
http://parafem.org.uk

http://www.amazon.com/Programming-Finite-Element-Method-Smith/dp/1119973341

Open Source Innovation Pipeline



Source: Margetts L. “Generating Wealth from Open Source Software”, MBA Dissertation, University of Manchester, 2011


ParaFEM Open Source Library
Solvers
Maths libraries
MPI
OpenMP
GPUs
Xeon Phi
ARM
Cloud

Random field generator

OpenFOAM FSI

ParaView Viz

Cellular Automata

ParaFEM Open Source Library

Solvers | Maths libraries | MPI | OpenMP

GPUs | Xeon Phi | ARM | Cloud

ABAQUS UMAT/UEL

ENSIGHT

Problem-driven Development Philosophy

Research Question or Engineering Problem

- Is HPC required to solve the problem?
- Does the existing software need customization?

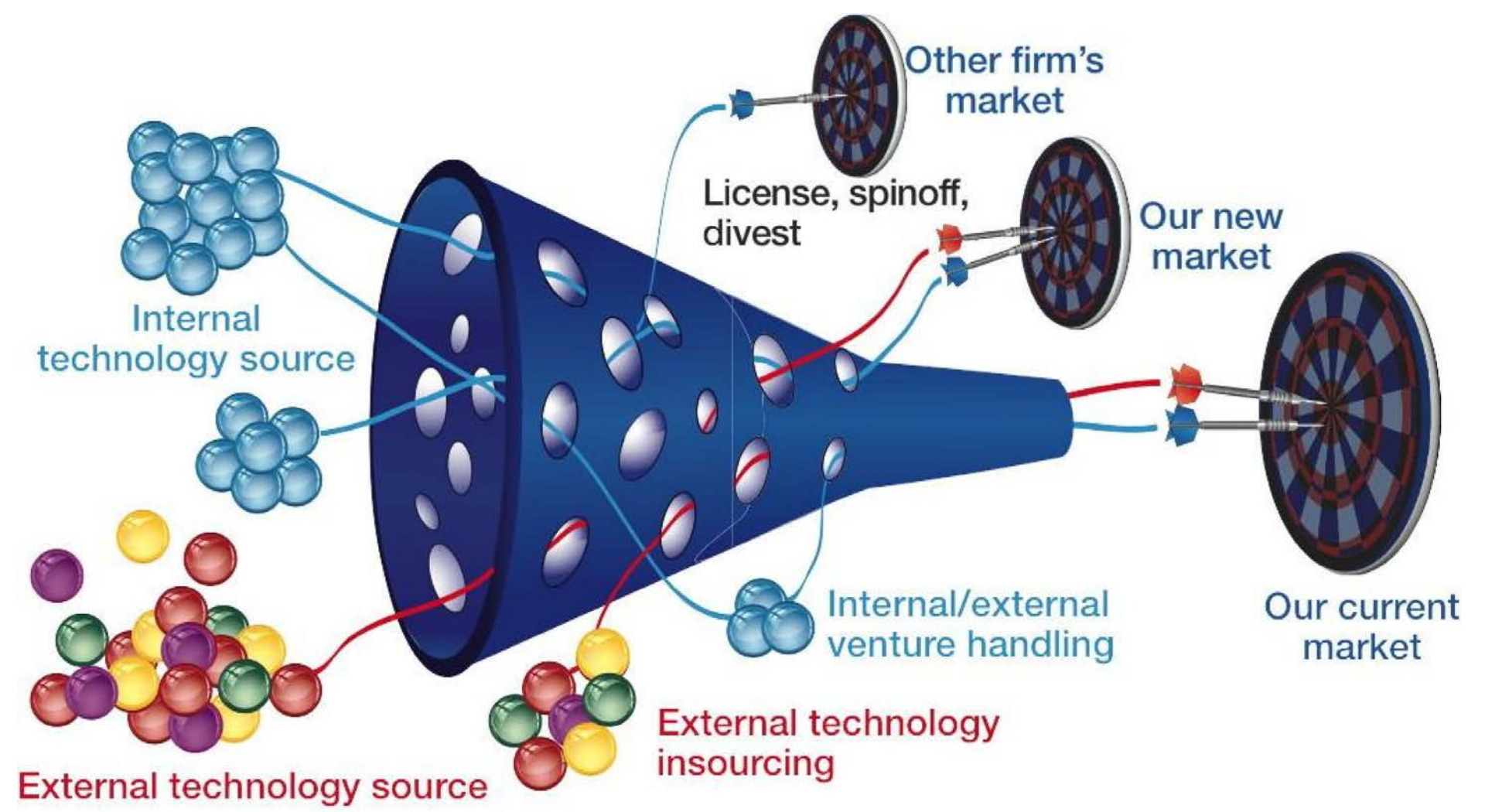
Implementation

- Test using analytical problem
- Compare with ISV software. If differences, fix or explain

Sustainability

- Source code committed to repository
- Publish modifications

Innovation

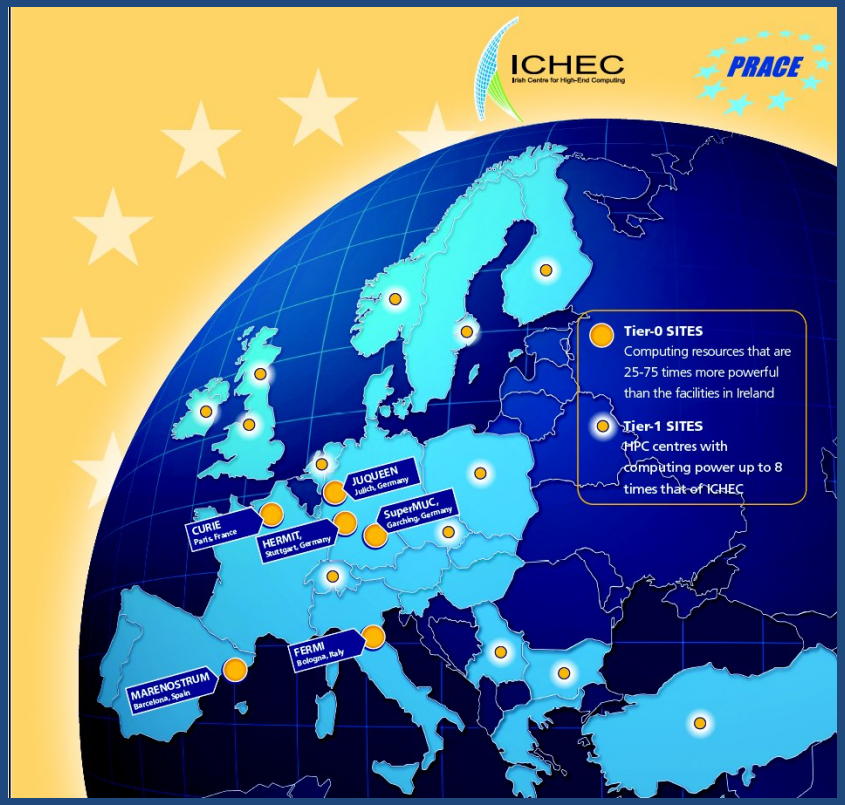


Exascale prototype
High risk
Open source
Research-driven

2015

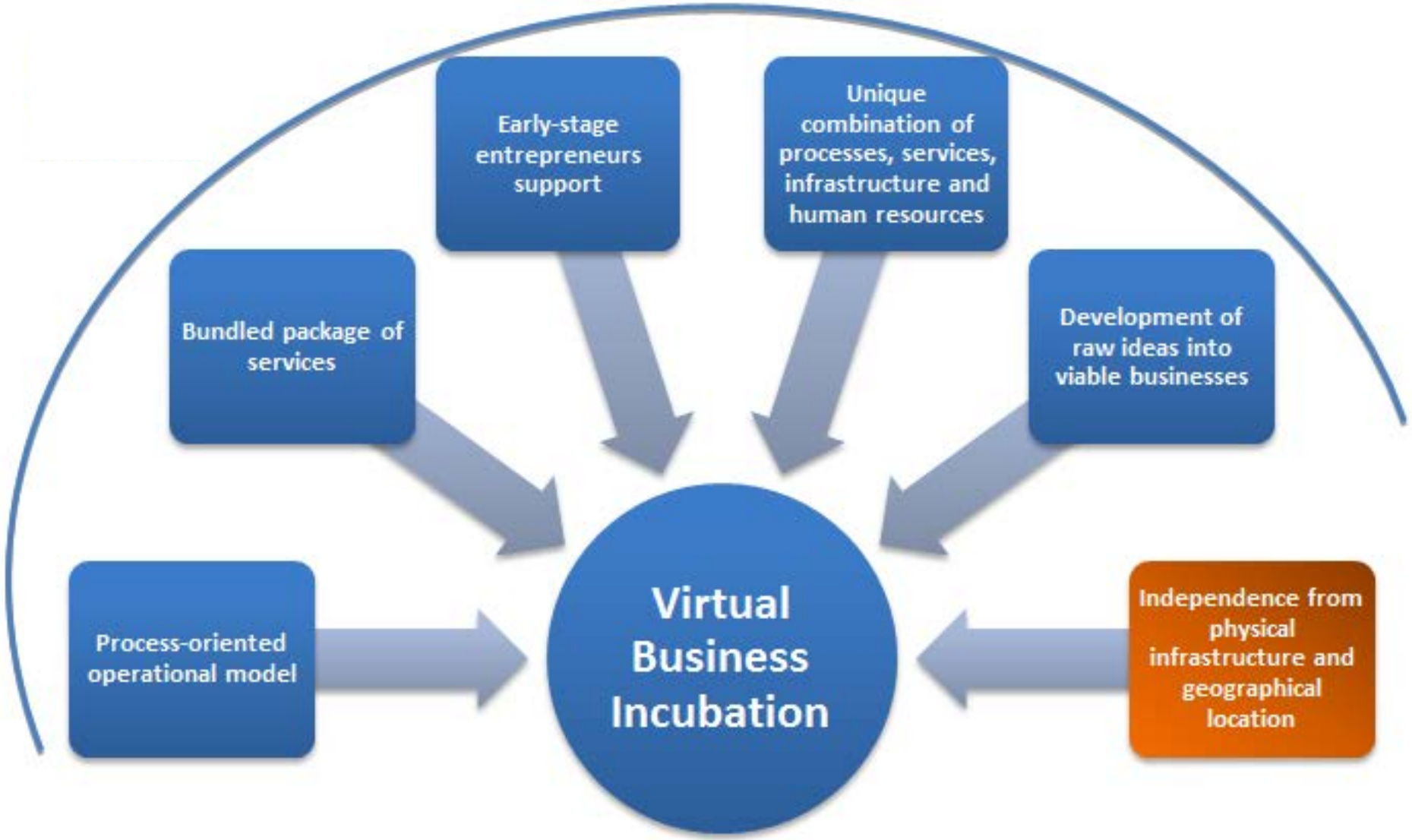
2030

Exascale desktop
Lower risk
ISV Products
Market-driven



- ✓Open calls for access
- ✓EU funded industrial engagement
- ✓National funded engagement
- ✓SME programmes
- ✓Large firms

Nurture the most fragile parts of the ecosystem
Encourage micro-firms, spin-out companies and OSS HPC service companies and innovative HPC products



Can PRACE be a virtual incubator for HPC spin out companies?

Image source: https://worldbusinessincubation.wordpress.com/

PRACEDAYS 2015 - Wednesday 1530-1800

"Establishing HPC computational environments in industry: a view from inside"

Dr Stefano Cozzini, CEO eXact Lab

"On the impact of automatic parallelization in technical computing for science and industry"

Manuel Arenaz, Appentra Solutions

"Opening access to HPC to all through the Constellation engineering ecosystem"

Nicolas Tonello, Constelcom

Conclusions

Final Thoughts

- ✓ Exascale computing for industrial applications (in engineering) needs to support workflows, not just the heroic scaling of single applications
- ✓ Exascale computing “now” - is not a market for ISVs, so open source s/w platforms are needed until Exascale is nearly on the desktop
- ✓ “We” need to support technology spinouts and early adopters. PRACE could take the role of an “EU virtual incubator”

Exascale Workstation in 2030?

Source: engineering.com