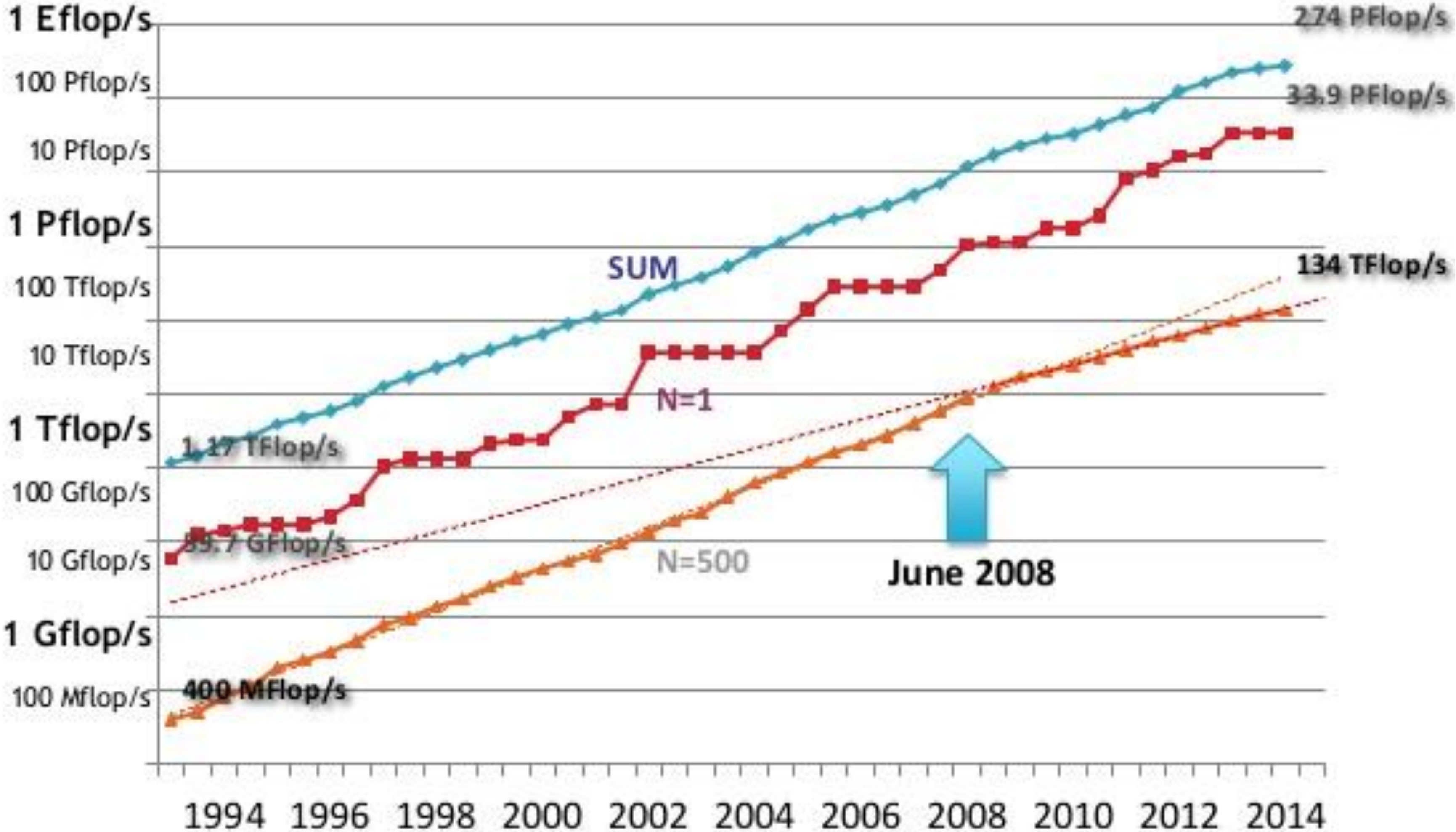
ParaFEM: A massively parallel alternative to Abaqus/Ansys for implicit solid mechanics

Dr Lee Margetts
School of Mechanical, Aerospace and Civil Engineering
http://parafem.org.uk

Advances in Hardware

Performance Development



Titan, Oak Ridge National Laboratory
20+ Petaflops

299,008 cores (Opteron) and 18,600 NVIDIA GPUs

>20,000,000,000,000,000 floating point operations per second


1,000,000,000,000,000,000
AN EXASCALE COMPUTER WILL PERFORM ONE QUINTILLION OPERATIONS PER SECOND.
An exascale computer can perform as many calculations per second as about 50 MILLION LAPTOPS.
Current projections for power consumption of exascale computers is put at 100 MEGAWATTS – the same amount of power as ONE MILLION 100-WATT lightbulbs.
AN EXASCALE COMPUTER WILL BE 1,000 TIMES FASTER than today's most powerful supercomputer: FUJITSU'S K COMPUTER.
Today's fastest supercomputers are GIGANTIC requiring space the size of a football field.
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.

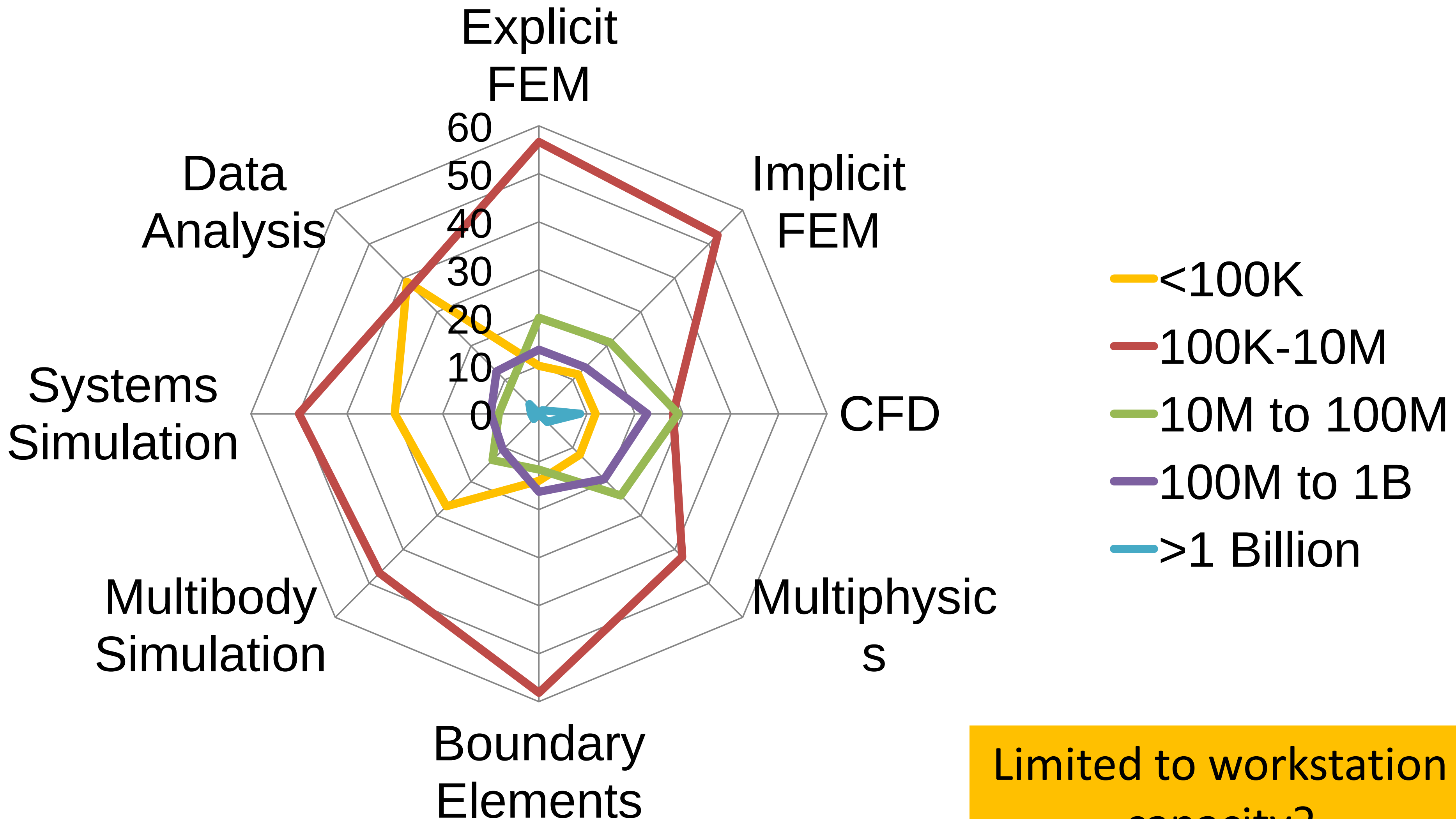
http://larreks.deviantart.com/art/Evolution-of-Tomb-Raider-425582963

#1 in 1996?

A8 Processor SoC
~172GFlops?

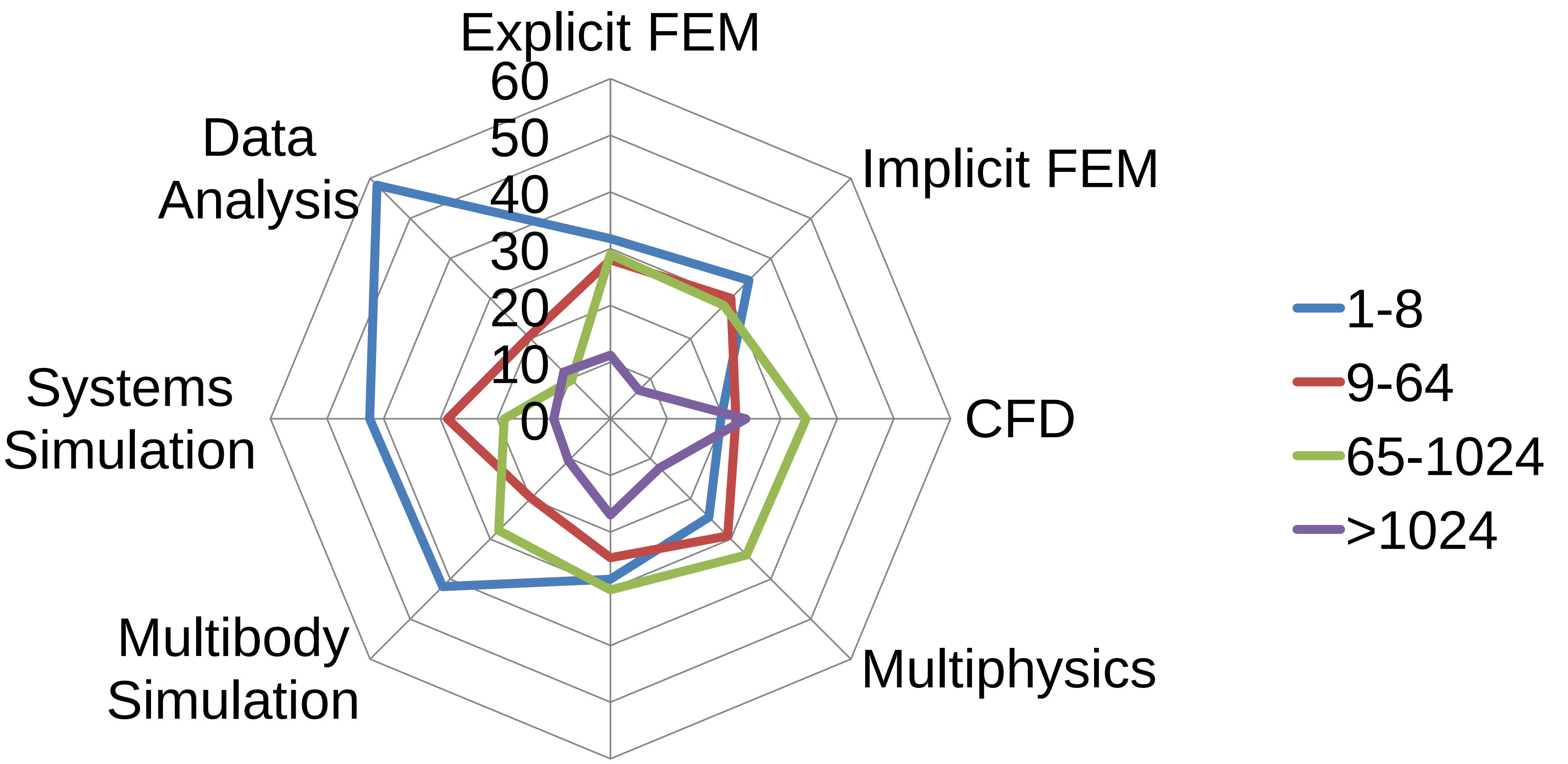
Engineering Simulation

NAFEMS Survey 2014 – Problem Size



Limited to workstation capacity?

NAFEMS Survey 2014 – Number of Cores



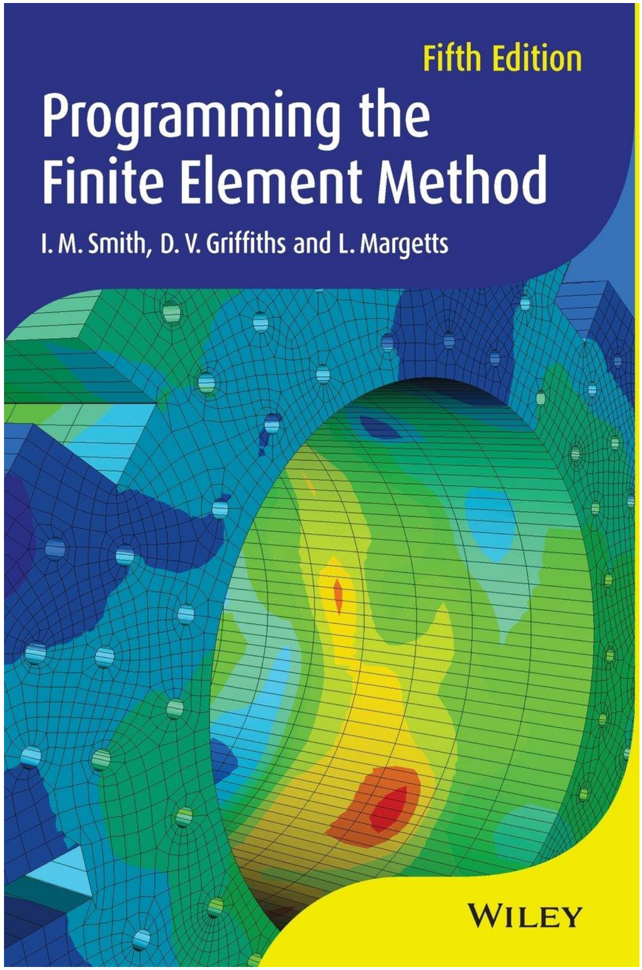
Limited to single compute node?

Large 3D finite element problems

Mesh Subdivision	Number of Equations
10 x 10 x 10	12,580
20 x 20 x 20	98,360
40 x 40 x 40	777,520
80 x 80 x 80	6,182,240
100 x 100 x 100	12,059,800
400 x 400 x 400	768,959,200
440 x 440 x 440	1,023,368,720

Tomography 4000 x 4000 x 4000 voxels = 10^{11} to 10^{12} dof

ParaFEM – General Purpose Parallel FE

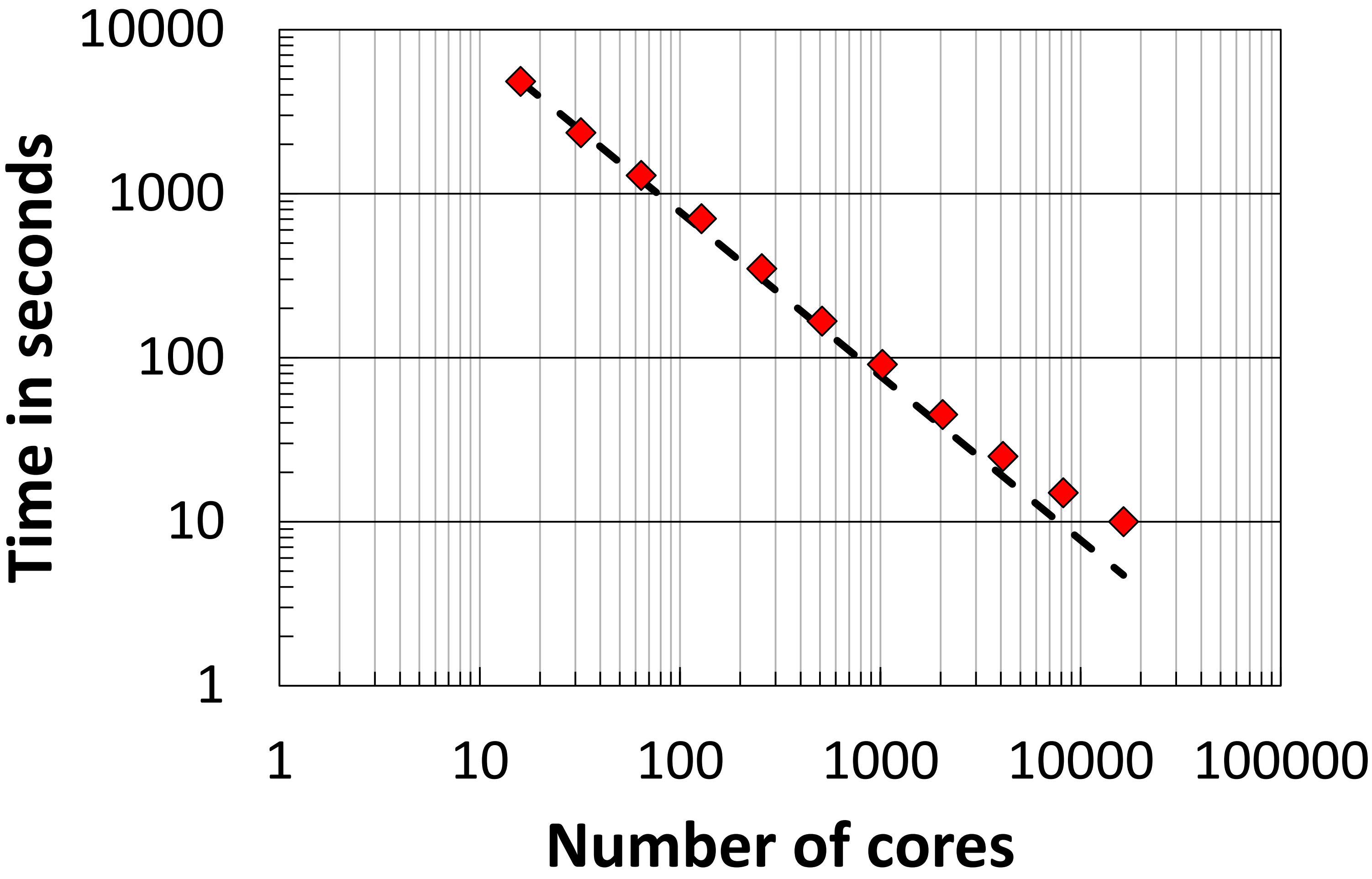


- Fortran + MPI
- Open source engineering package
- ~64,000 cores
- >1 billion degrees of freedom
- Similar functionality to Ansys, Abaqus
- Used for teaching and research
- 750+ registered on website
- ~1000 citations of text book
- http://parafem.org.uk
- http://www.amazon.com/Programming-Finite-Element-Method-Smith/dp/1119973341

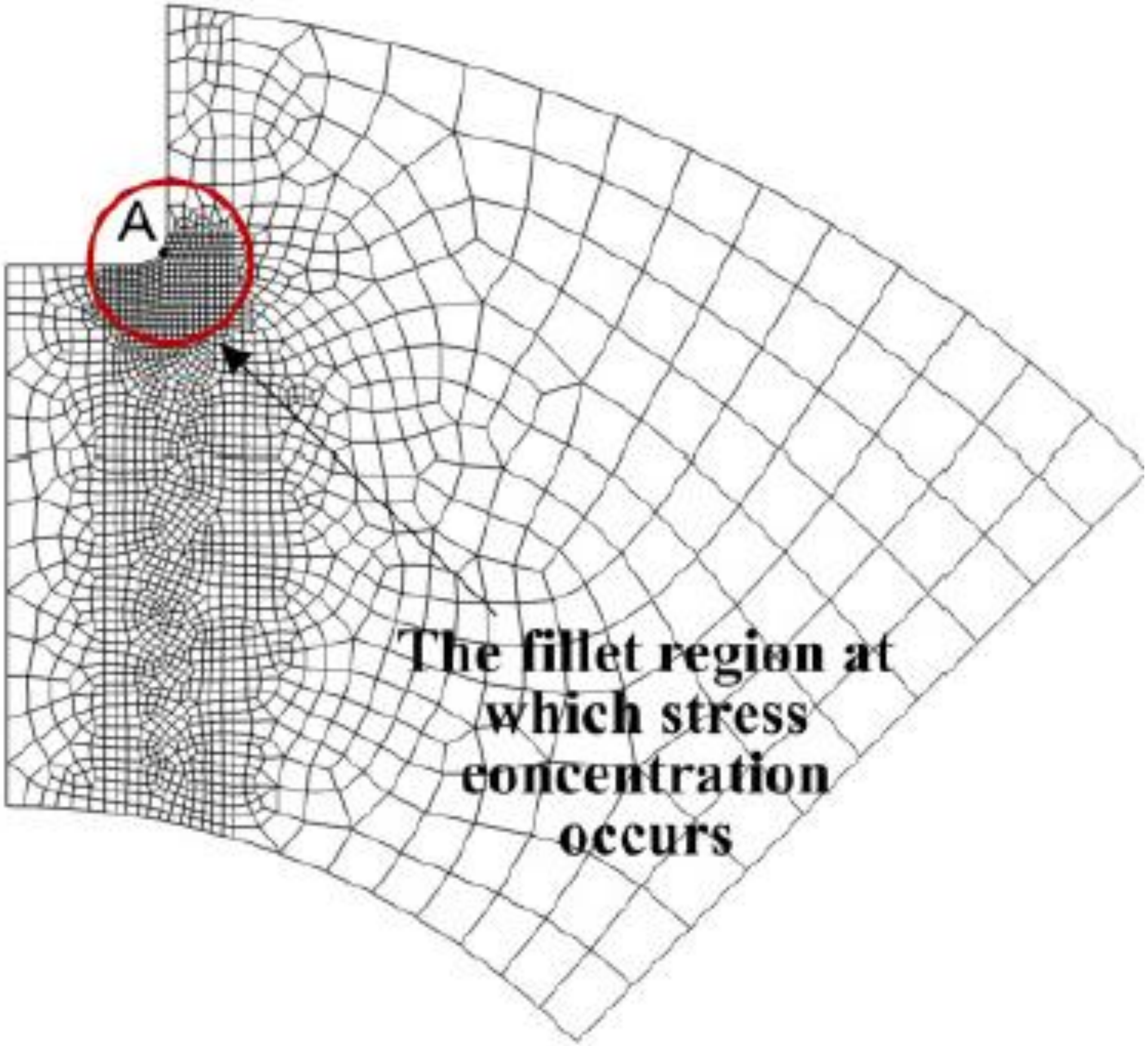
Time for one solution step - elasto-plasticity

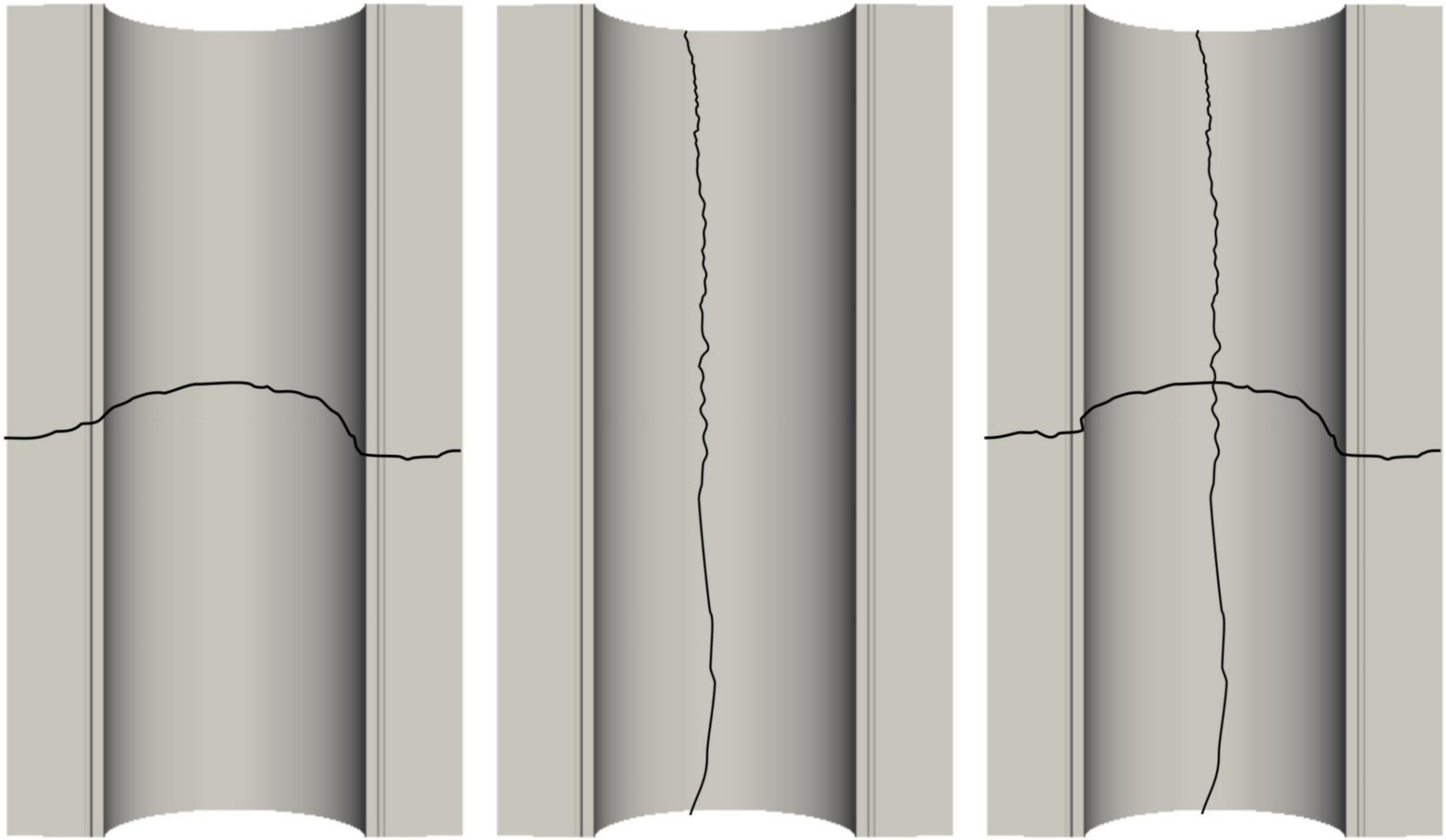
Mesh (equations)	Processes	Time (secs)
12,059,800	16	486
	32	256
	64	140
	128	83
768,959,200	1024	2721
	2048	1213
	4096	662

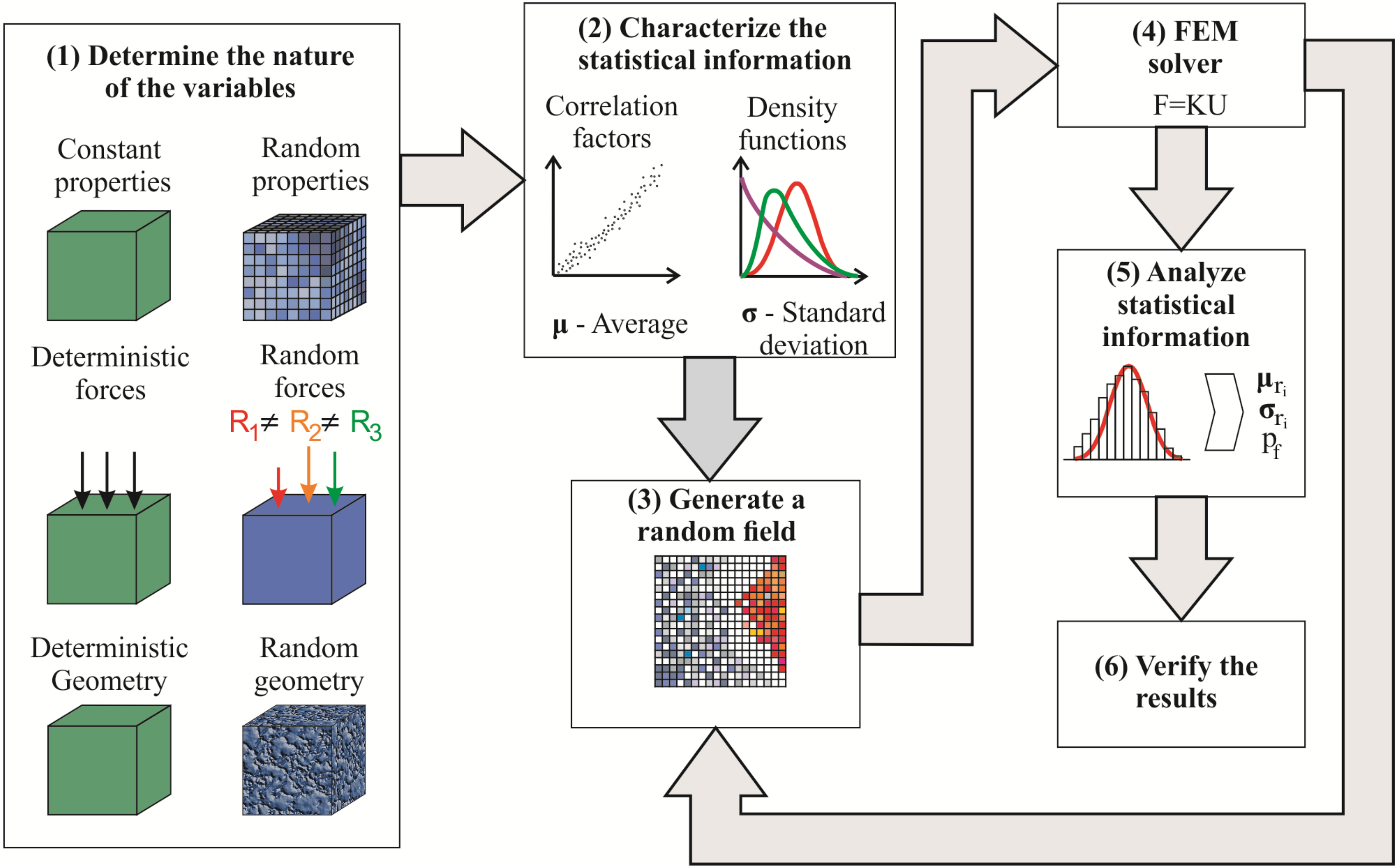
Time for one solution step – transient thermal



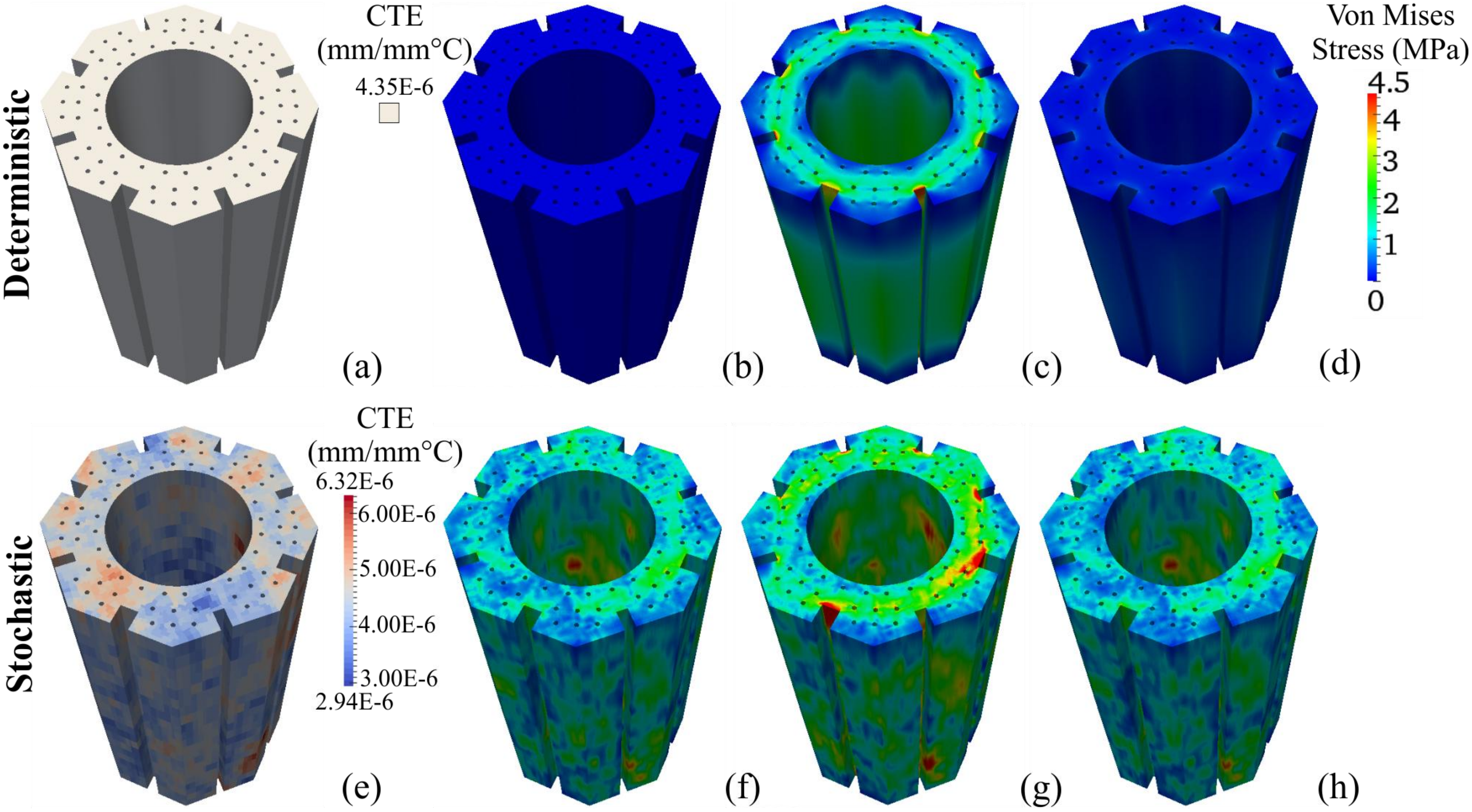
Monte Carlo Simulation

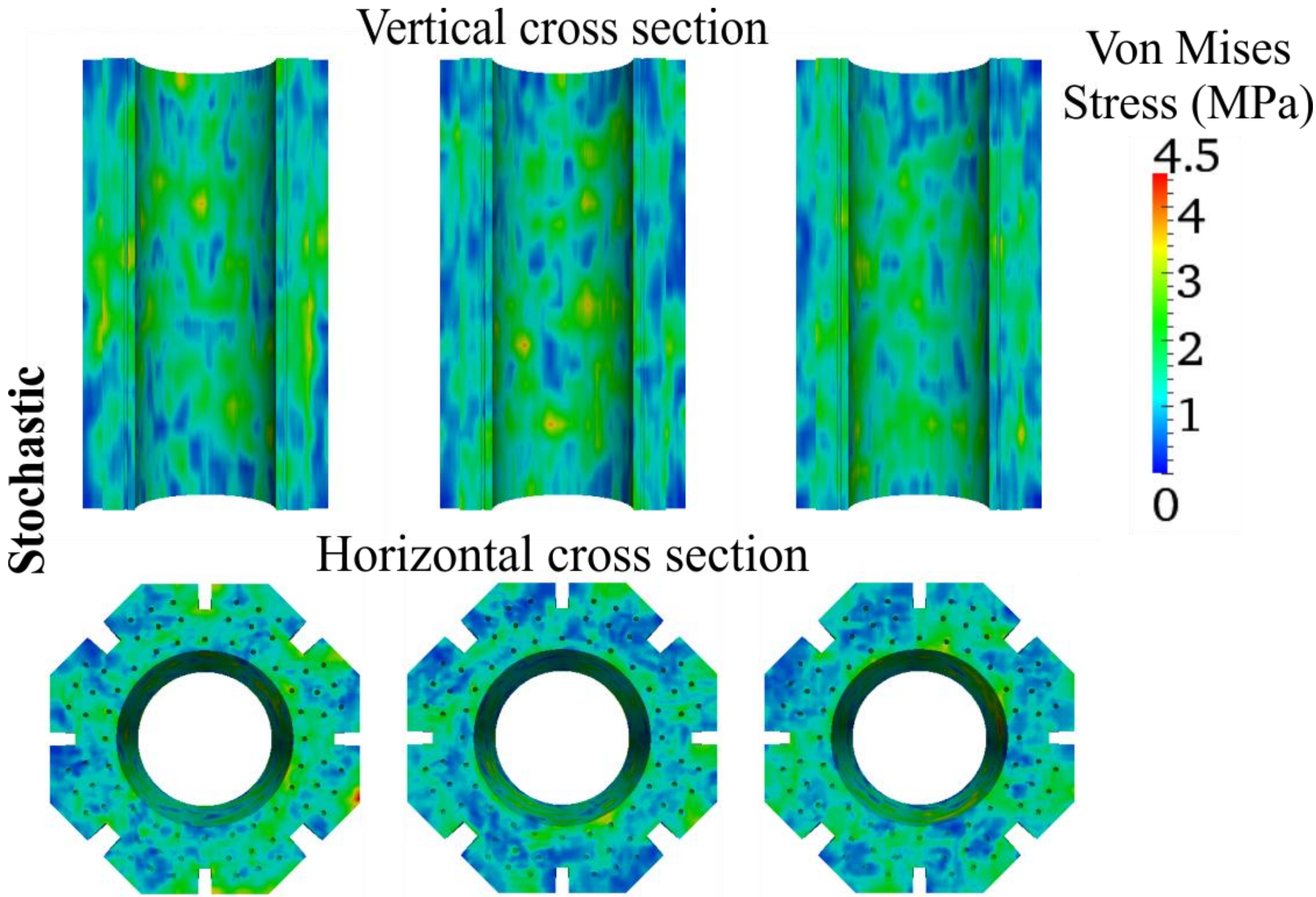

A
The fillet region at which stress concentration occurs





(1) Determine the nature of the variables
Constant properties
Random properties
Deterministic forces
Random forces
$R_1 \neq R_2 \neq R_3$
Deterministic Geometry
Random geometry
(2) Characterize the statistical information
Correlation factors
Density functions
μ - Average
σ - Standard deviation
(3) Generate a random field
(4) FEM solver
F=KU
(5) Analyze statistical information
μ_{r_i}
σ_{r_i}
p_f
(6) Verify the results


Deterministic
Stochastic
CTE
(mm/mm°C)
4.35E-6
CTE
(mm/mm°C)
6.32E-6
6.00E-6
5.00E-6
4.00E-6
3.00E-6
2.94E-6
Von Mises
Stress (MPa)
4.5
4
3
2
1
0
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)



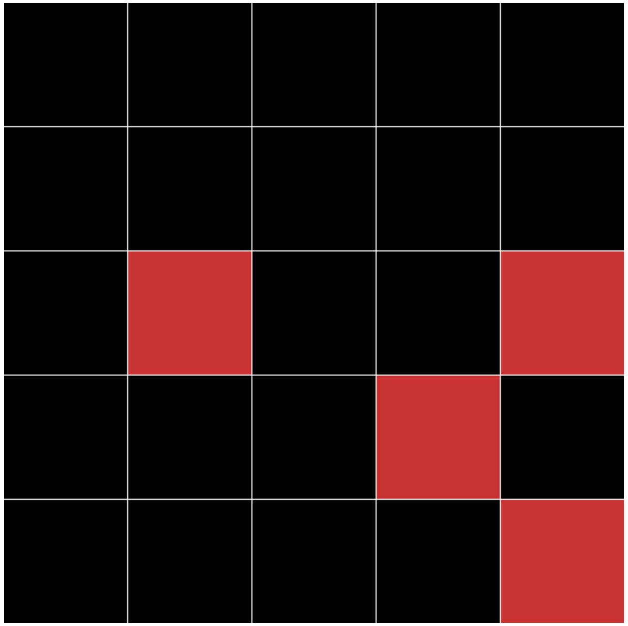
Vertical cross section
Von Mises
Stress (MPa)
4.5
4
3
2
1
0
Stochastic
Horizontal cross section

Multi-scale Simulation

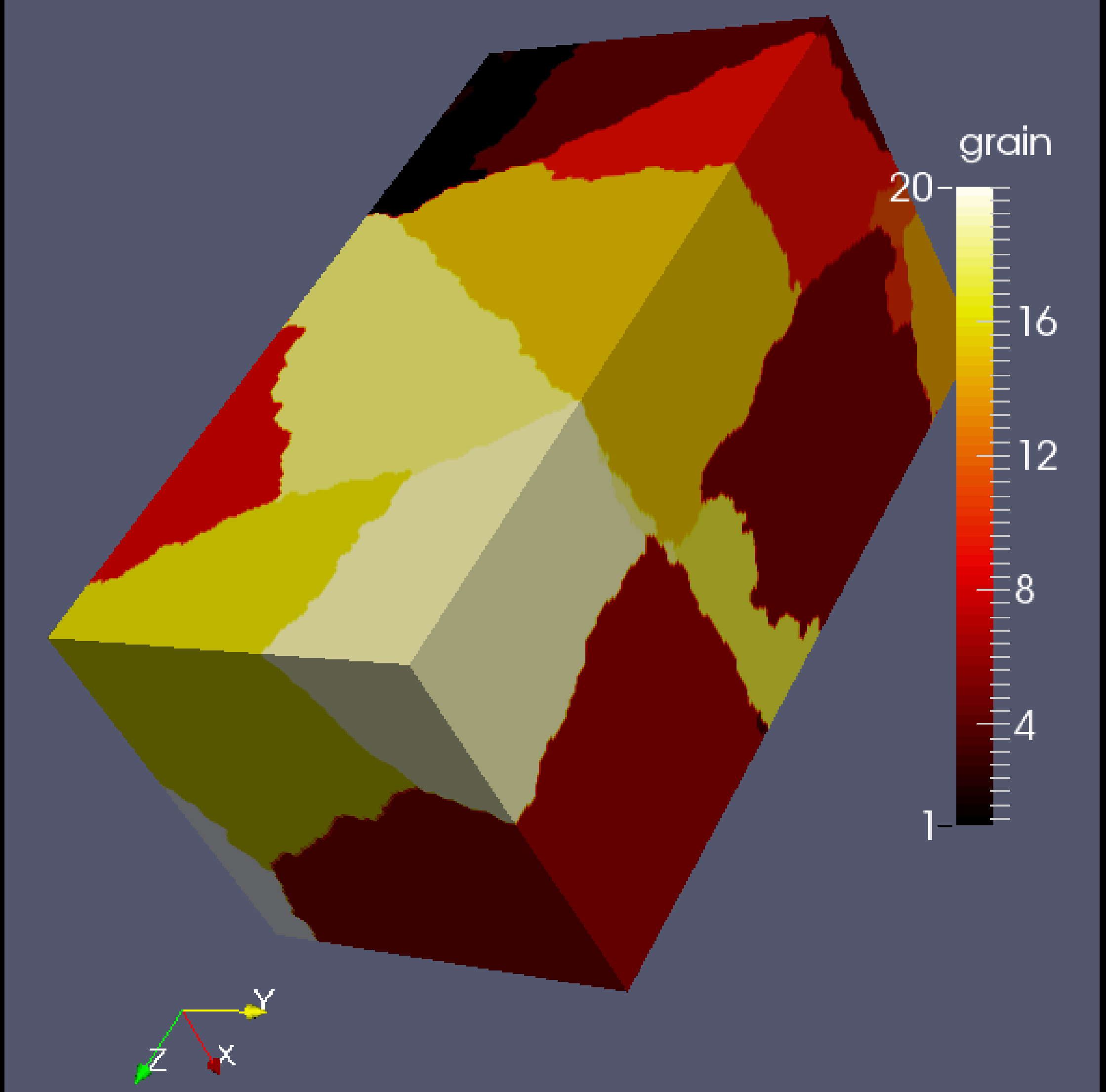
Meso-scale models

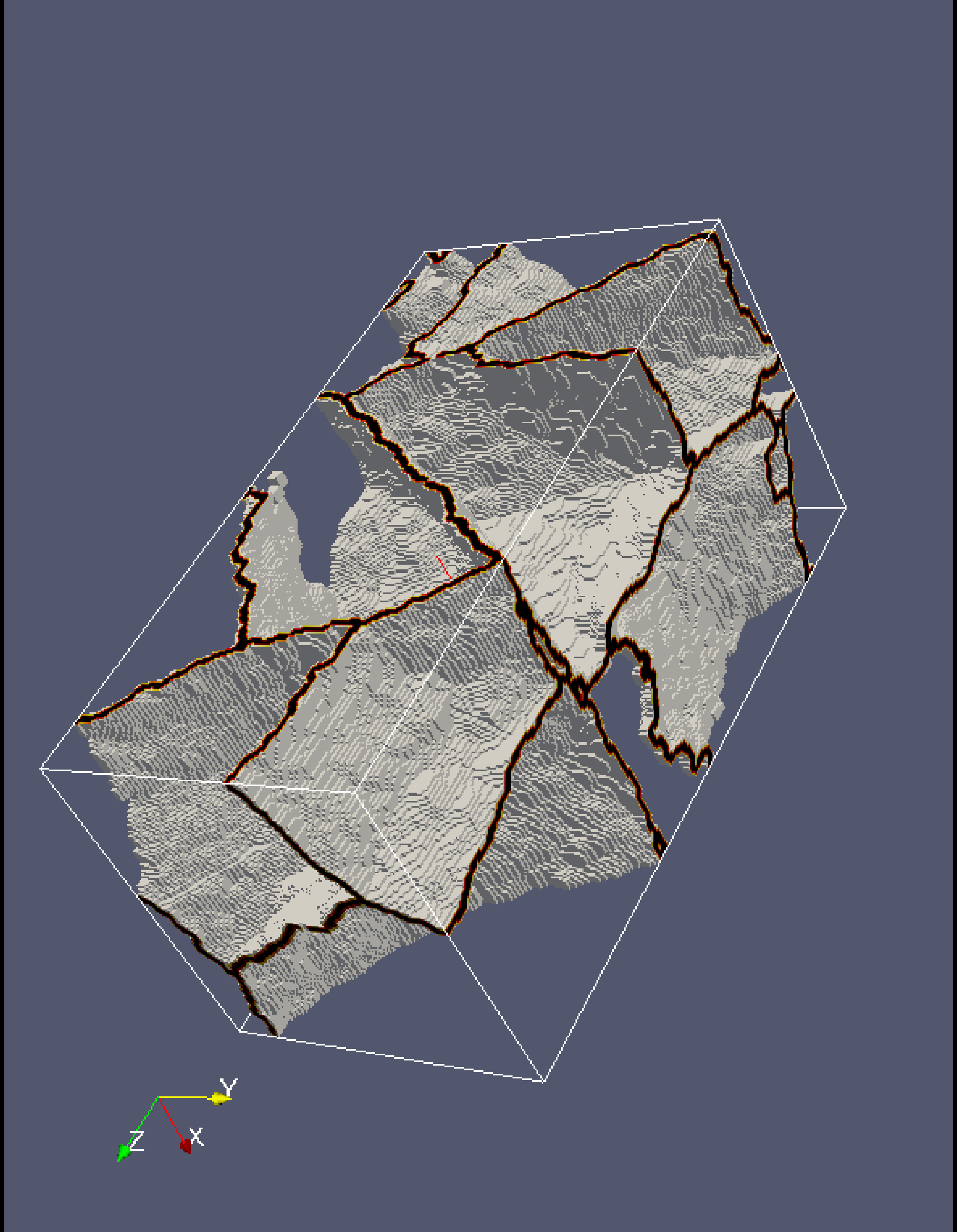
- Lattice-based or cellular automata ...
- Simulate mechanisms at grain scale
- Emergent behaviour such as fatigue/fracture
- Iterative 2-level process
  – Meso-scale updates FE scale continuum properties
  – FE computes new stresses

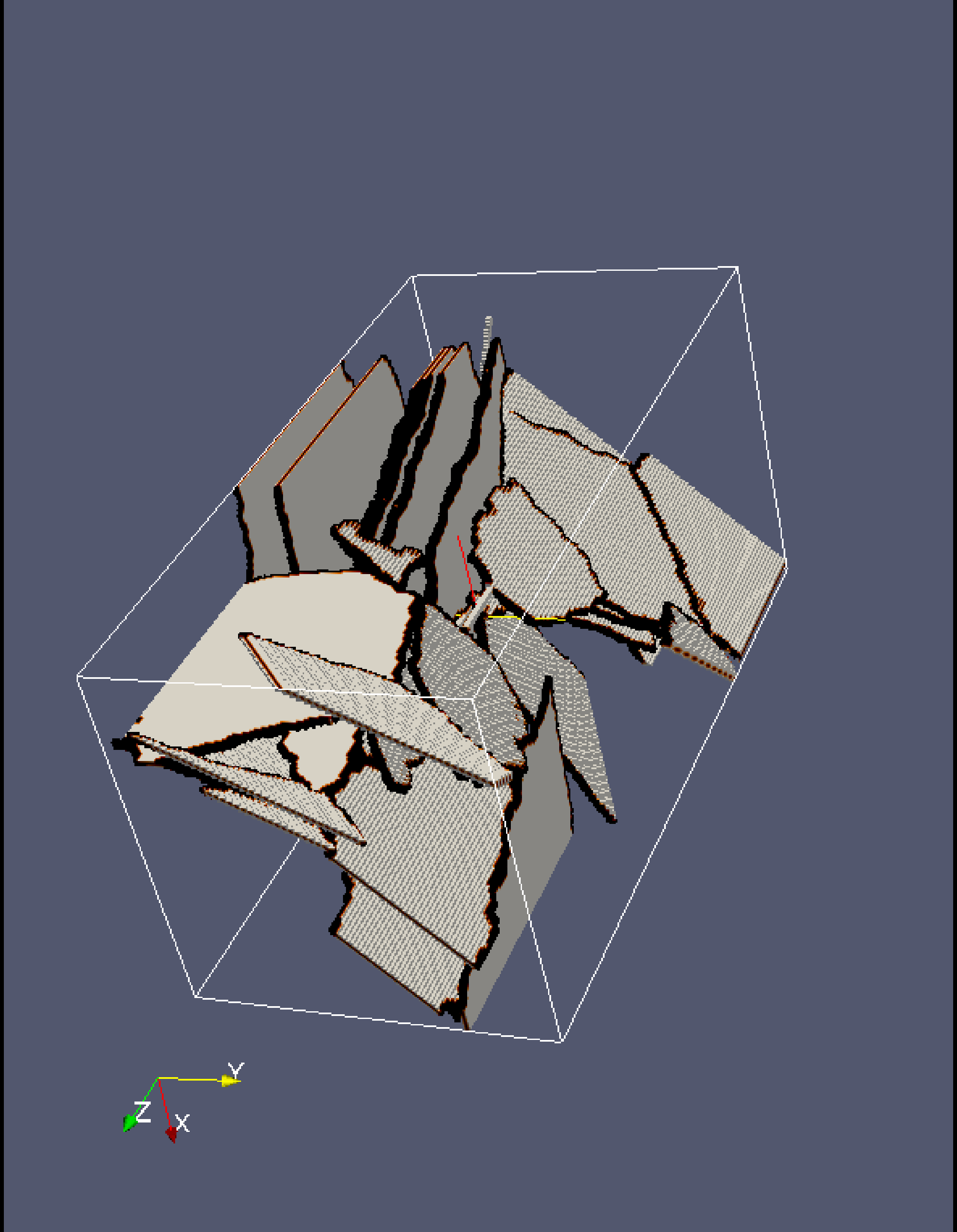
Cellular automata



Shterenlikht A. and Howard I.C. (2006) “The CAFE model of fracture – application to a TMCR steel”, Fatigue and Fracture of Engineering Materials and Structures, Volume 29, Issue 9-10


grain
20
16
12
8
4
1
Y
Z
X


Y
Z
X



Y
Z
X

Multiphysics

ALSTOM

EPSRC CASE PhD Studentship

Couple OpenFOAM + ParaFEM

Fluid-structure interaction in wind farms

MANCHESTER
1824
The University of Manchester
Aerospace Research Institute

PhD Student in cohesive fracture
Modelling damage in CFC
Abaqus UEL interface in ParaFEM

Other Activities

THE UNIVERSITY *of* EDINBURGH

Nonlinear geometry with plasticity
Abaqus UMAT interface

User Upgrade Program
Available TODAY

Intel® Xeon Phi™ Product Family

Industry and User Momentum

1 TFLOPS[1]

Knights Corner

Intel® Xeon Phi™ Coprocessor – Applications and Solutions Catalog

3+ TFLOPS[2]

-Bootable Processor
-On-Pkg, High BW Memory
-Integrated Fabric

Knights Landing

2H'15
First Commercial Systems

>50 systems providers expected[3]

\+

many more *card-based systems*

>100 PFLOPS *customer system compute commits to-date*[3]

Announcing

Knights Hill

3rd Generation Intel® Xeon Phi™ Product Family

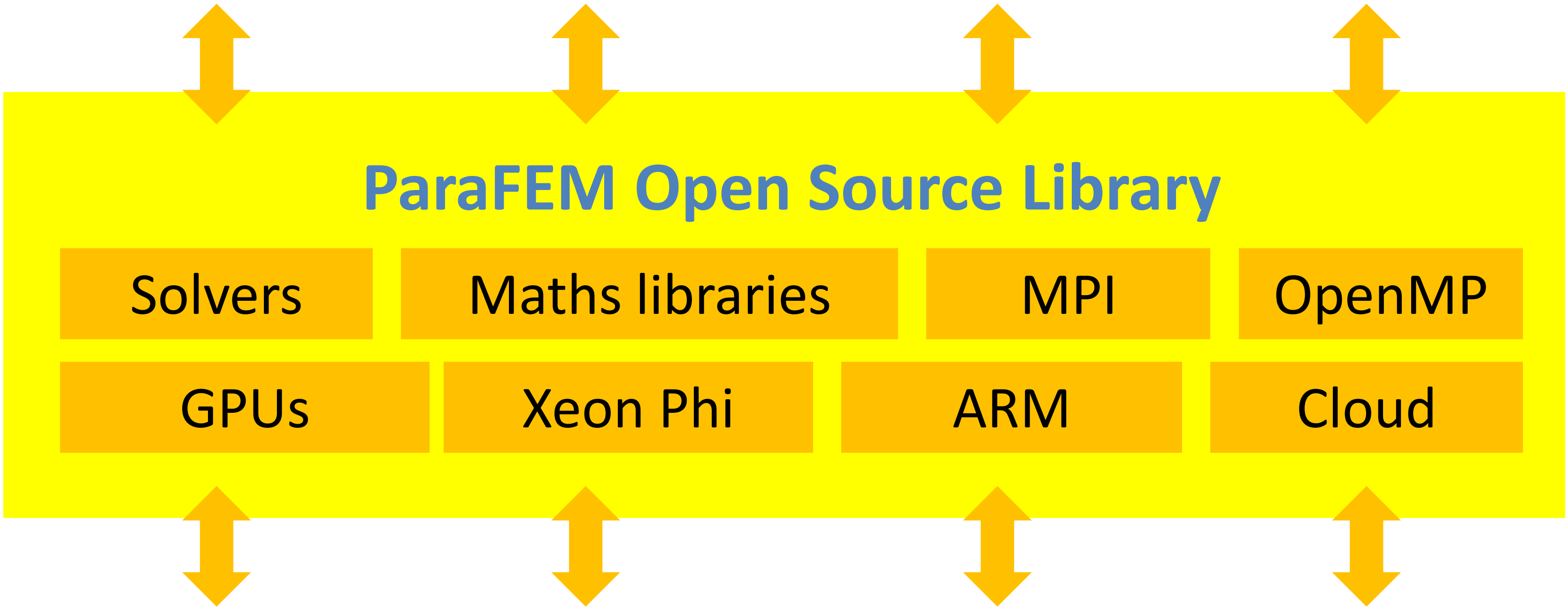
2nd Generation Intel Omni-Path Architecture

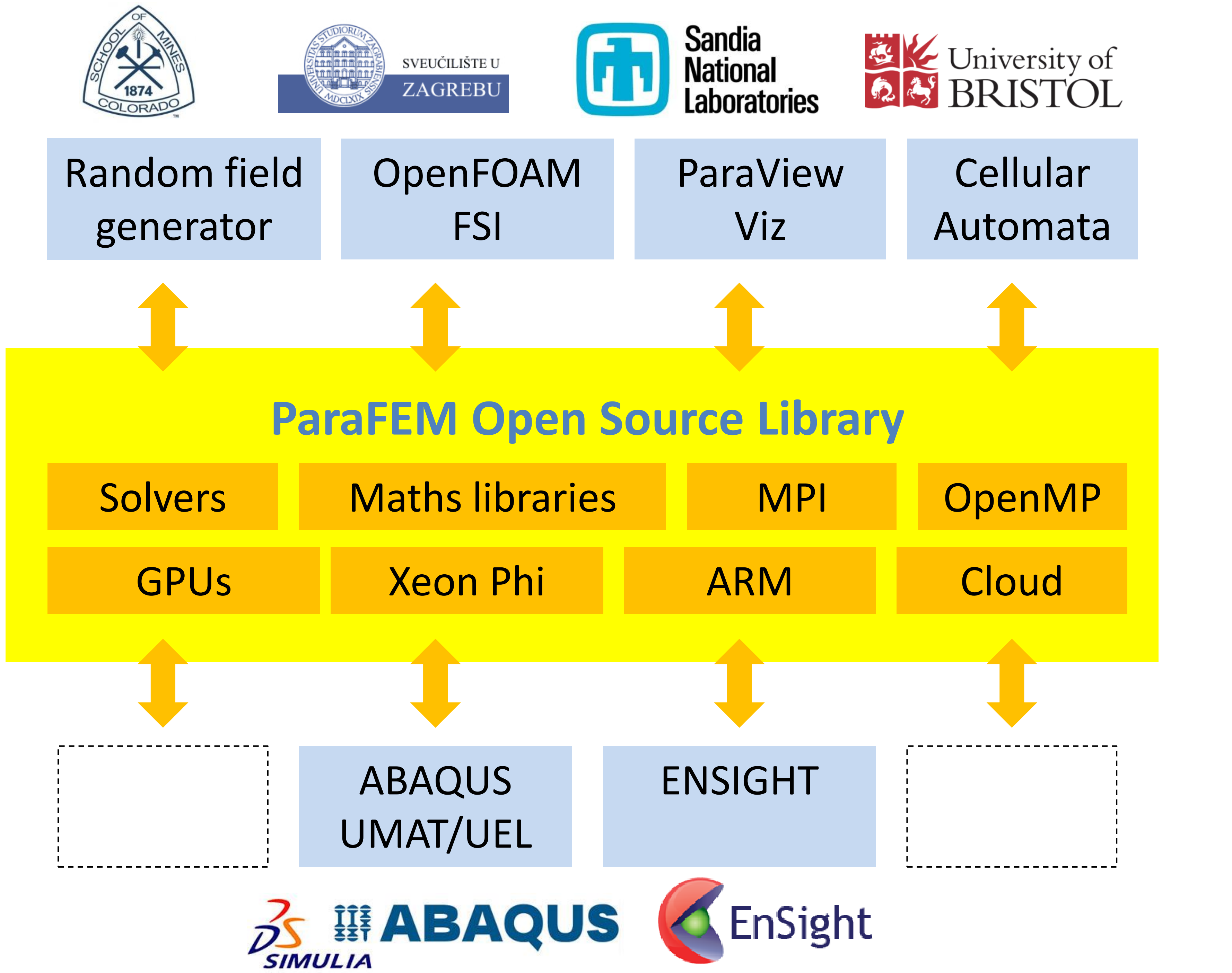
10nm process technology

[1] Claim based on calculated theoretical peak double precision performance capability for a single coprocessor. 16 DP FLOPS/clock/core * 61 cores * 1.23GHz = 1.208 TeraFLOPS
[2] Over 3 Teraflops of peak theoretical double-precision performance is preliminary and based on current expectations of cores, clock frequency and floating point operations per cycle. FLOPS = cores x clock frequency x floating-point operations per second per cycle. [3] Intel internal estimate

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

Summary


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

Summary

- Aiming to build the next generation platform for engineering simulation ~2018-2020
- Software engineering focus on “plug and play” interfaces between OSS/proprietary code
- No need to reinvent the wheel
- Development work is research-driven
- Strong interest from industry, USA and China