On substitution of commercial FE codes with an in-house solution for real-world problems: A short review on the competition between ease-of-use and speed

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Outline

Introduction & Motivation

User intervention of ABAQUS vs. in-house FE code 4C

Performance comparison ABAQUS vs. in-house FE code 4C

Further development of in-house FE code 4C

Conclusion

Introduction

Helmholtz Association (18 centers)

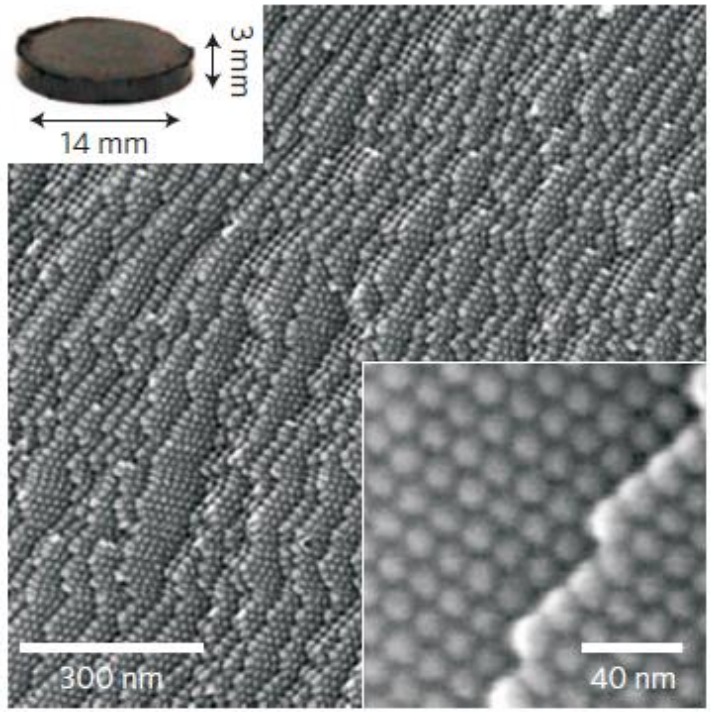
Helmholtz-Zentrum Hereon (15 Institutes, 1100 employees)

Motivation

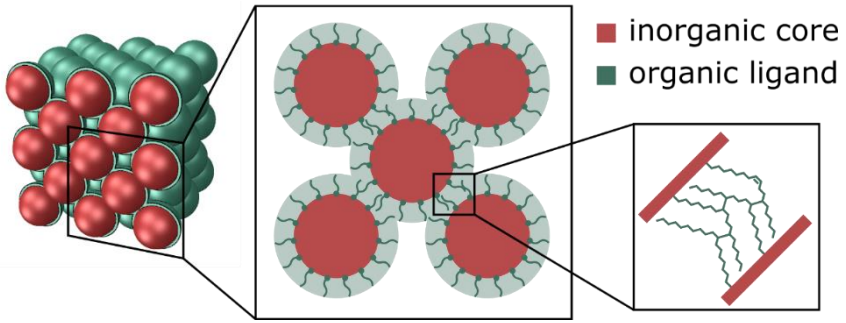
Composite (targets on high stiffness, hardness, and strength) based on

- **ceramic nanoparticles with very high volume content (>50%) in a crystalline arrangement**
- **surrounded by thin organic layer**
- **particle diameter ~20 nm**
- **organic layer thickness ~ 2 nm**

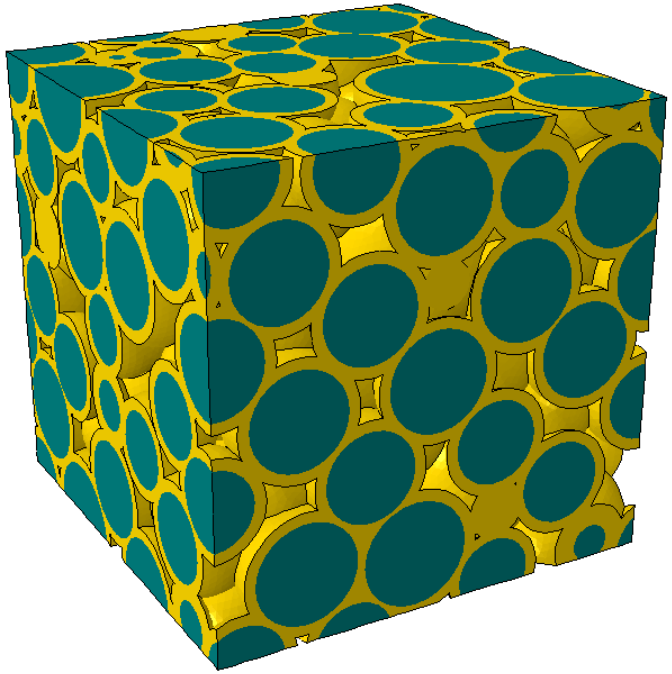
Real material
(scanning electron microscope)



Modeling assumption



FE model (geometry)



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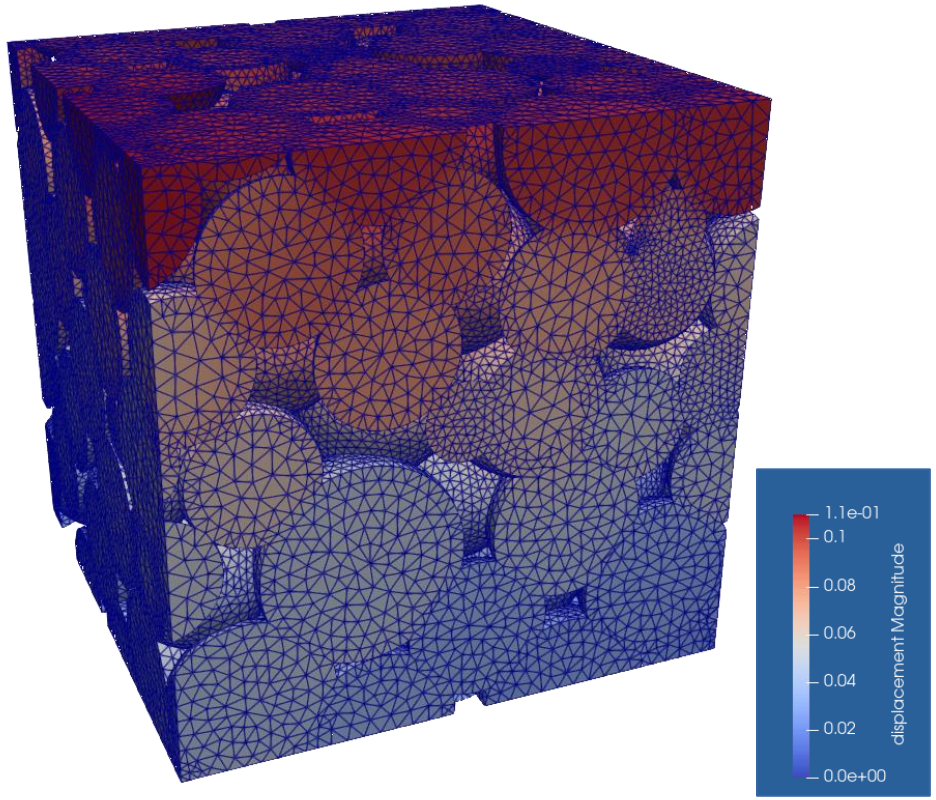
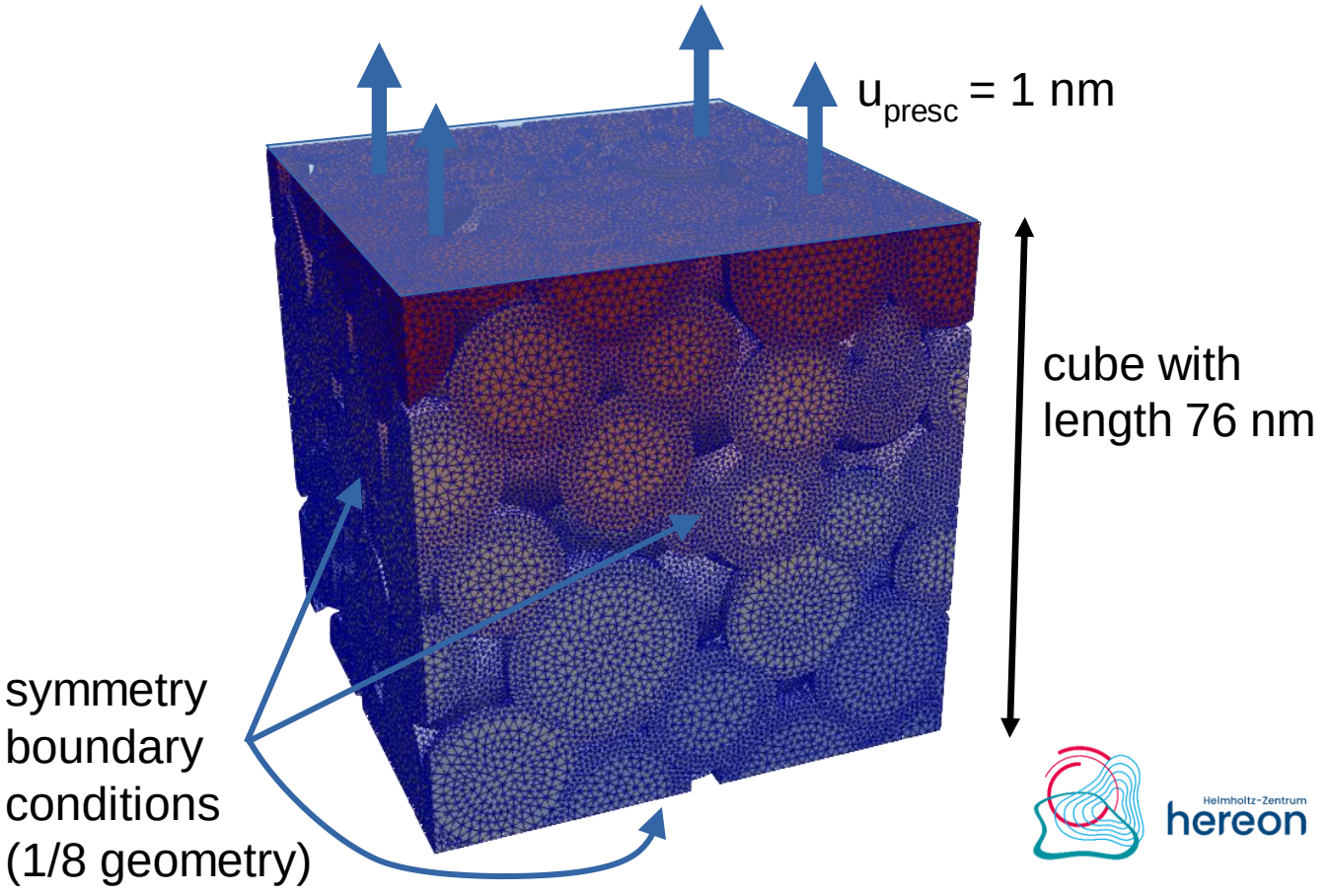
Simulation of a microstructural cell: FE models

	# Nodes	# Elements	# DOF	Material 1 (particle)	Material 2 (organic layer)
Small model (650k)	216,768	1,161,671 (tet4)	650,304	E = 163000 MPa v = 0.3	E = 13000 MPa v = 0.48
Large model (17M)	5,851,079	4,215,573 (tet10)	17,553,237		





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Transition phase from commercial FE solver to in-house code 4C at Hereon

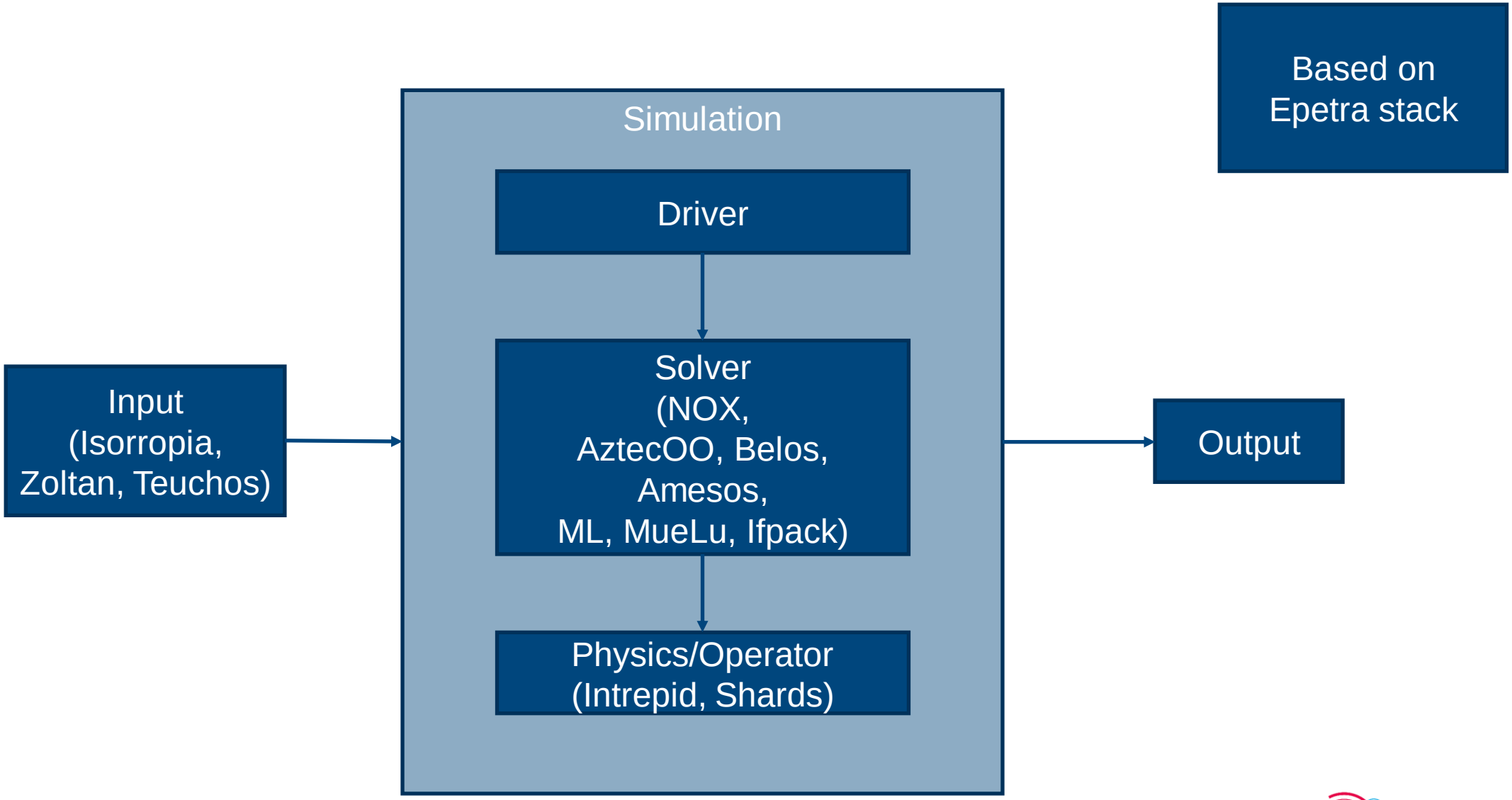
- Long-term experience with ABAQUS and UMAT (User Subroutines) implementations for material modeling
- Transition phase started towards in-house FE solver 4C
- Challenges/opportunities with in-house code (based on Trilinos solvers)
  - Just little knowledge about mathematical background of linear solvers of many co-workers (so far focus on material modeling)
  - How to use full potential of available linear solvers?
  - How to obtain good solver parameters for fast convergence?

Commerical code: ABAQUS

- Documentation of ABAQUS internal details sparse
  - Iterative linear solver using preconditioned Krylov method (CG)
  - Preconditioner is calculated only once at the beginning of each linear system solve (“PAMG”)
  - Hybrid MPI & thread-based parallelization

- User intervention very limited: available options are
  - Relative tolerance of convergence (default 10^{-6})
  - Maximum number of linear solver iterations (default 500)

Usage of Trilinos within our in-house code 4C



In-house code 4C
Solver options: GMRES, ILU

```
SOLVER          Aztec_MSR
AZSOLVE         GMRES
AZTOL           1.0E-6
AZCONV          AZ_r0
AZITER          500
AZSUB           50
AZPREC          ILU
IFPACKGFILL     2
```

In-house code 4C
Solver options: GMRES, AMG using Chebychev smoother

SOLVER	Aztec_MSR
AZCONV	AZ_r0
AZITER	500
AZOMEGA	0
AZPOLY	5
AZPREC	ML
AZREUSE	5
AZSOLVE	GMRES
AZSUB	50
AZTOL	1e-06

ML_AGG_SIZE	27
ML_COARSEN	UC
ML_DAMPCOARSE	1
ML_DAMPFINE	0.59
ML_DAMPMED	0.69
ML_MAXCOARSESIZE	1000
ML_MAXLEVEL	5
ML_PROLONG_SMO	1.33
ML_PROLONG_THRES	0
ML_SMOOTHERCOARSE	KLU
ML_SMOOTHERFINE	CHEBYCHEV
ML_SMOOTHERMED	CHEBYCHEV
ML_SMOTIMES	9 9 9 9 1

In-house code 4C
Solver options: GMRES, AMG using SGS smoother

SOLVER	Aztec_MSR
AZCONV	AZ_r0
AZITER	500
AZOMEGA	0
AZPOLY	5
AZPREC	ML
AZREUSE	5
AZSOLVE	GMRES
AZSUB	50
AZTOL	1e-06

ML_AGG_SIZE	27
ML_COARSEN	UC
ML_DAMPCOARSE	1
ML_DAMPFINE	0.59
ML_DAMPMED	0.69
ML_MAXCOARSESIZE	1000
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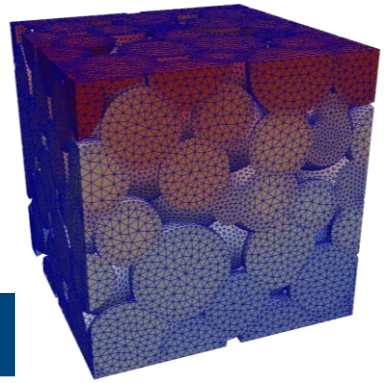
ML_PROLONG_SMO	1.33
ML_PROLONG_THRES	0
ML_SMOOTHERCOARSE	KLU
ML_SMOOTHERFINE	SGS
ML_SMOOTHERMED	SGS
ML_SMOTIMES	3 3 3 3 1

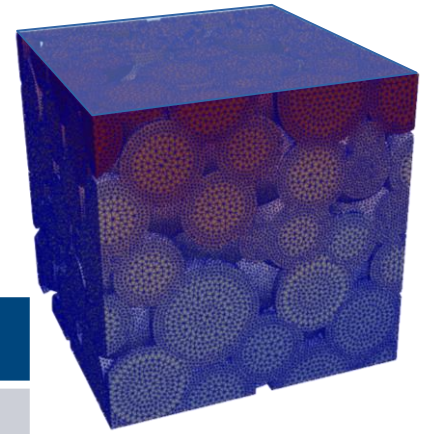
Wall clock timings in sec microstructural cell (small model 650k)



# CPUs	8	16	32	64	128
ABAQUS, direct, MPI	42 (1)	37 (1)	34 (1)	53 (1)	
ABAQUS, iterative, MPI	65 (2)	64 (2)	13 (2)	11 (2)	
4C, direct, MPI			1440	761	
4C, GMRES, ILU	33.2 (1)	20.1 (1)	13.1 (1)	8.3 (1)	10.4 (1)
4C, GMRES, AMG (Cheb.)	24.5 (1)	16.8 (1)	12.6 (1)	9.9 (1)	8.0 (1)
4C, GMRES, AMG (SGS)	16.3 (2)	18.0 (7)	28.0 (12)	4.6 (2)	2.0 (1)

In parentheses: number of Newton iterations necessary

Wall clock timings in sec microstructural cell (large model 17M)



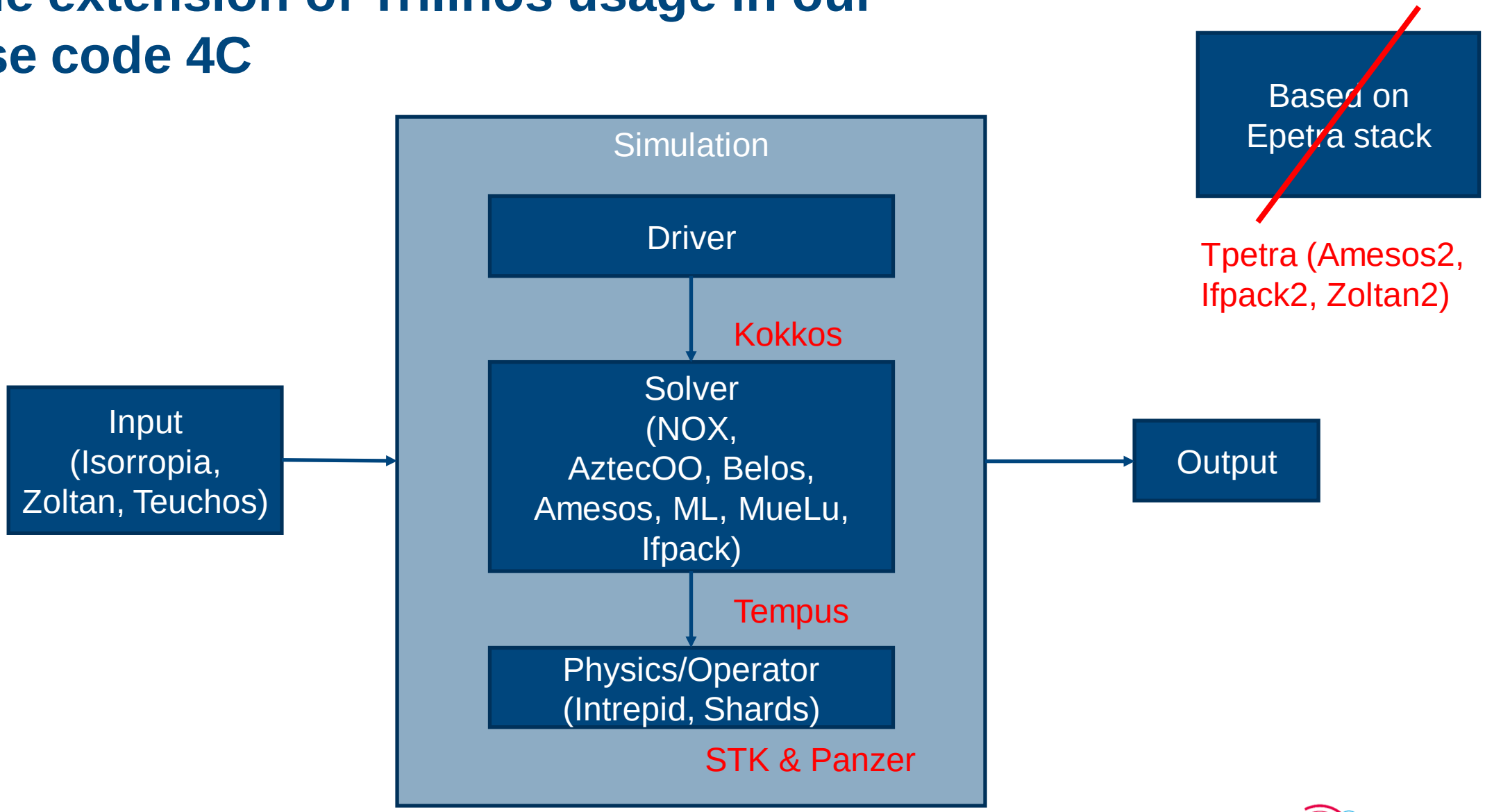
# CPUs	32	64	128
ABAQUS, iterative, MPI	227 (2)	212 (2)	220 (2)
4C, GMRES, ILU	1417 (1)	706 (1)	331 (1)
4C, GMRES, AMG (Cheb.)	918 (1)	229 (2)	266 (1)
4C, GMRES, AMG (SGS)	*	71 (1)	336 (6)

In parentheses: number of Newton iterations necessary

*Some solver iterations did not converge, simulation aborted after >1 hour…

ABAQUS' direct solver needs exhaustive time for such a large model (> 1 hour)

Possible extension of Trilinos usage in our in-house code 4C



Conclusion

- Transition from commercial FE solver to (Trilinos based) in-house FE solver leads to challenges in prescribing additional parameters especially for linear solver
- Choosing good parameters necessary to achieve at least same level of performance compared to commercial FE solver
- Extension of Trilinos usage in our in-house FE solver under consideration