Multi-level μ-Finite Element Analysis for Human Bone Structures

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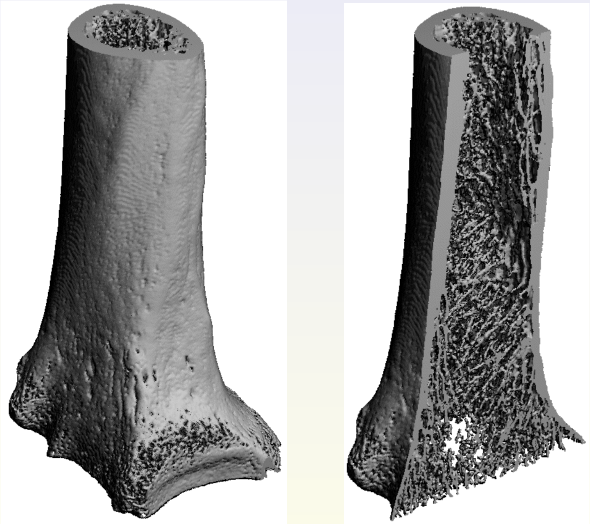
Outline of the talk

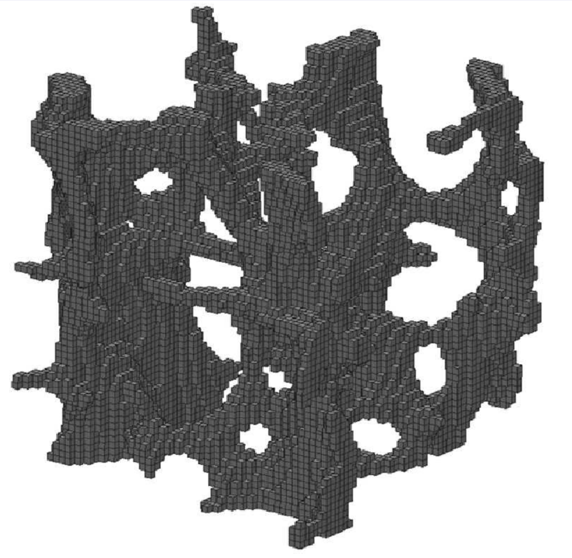
1. The need for μFE analysis of bones
2. Mathematical formulation
3. Solving the system of equations
4. The Trilinos Software framework
5. Numerical experiments

The need for μFE analysis of bones

- *Osteoporosis* is disease characterized by low bone mass and deterioration of bone microarchitecture.
- Lifetime risk for osteoporotic fractures in women is estimated close to 40%; in men risk is 13%
- Enormous impact on individual, society and health care social systems (as health care problem second only to cardiovascular diseases)
- Since global parameters like bone density do not admit to predict the fracture risk, so patients have to be treated in a more individual way.
- Today's approach consists of combining 3D high-resolution CT scans of individual bones with a micro-finite element (μFE) analysis.



Distal part (20% of the length) of the radius in a human forearm.
Cortical vs. trabecular bone.



Computational domain consists of the union of equal (micro) cubes. Obtained by means of CT scan.

Mathematical formulation

- Equations of linear elasticity (weak formulation):
  Find $\mathbf{u} \in [H^1_E(\Omega)]^3 = \{v \in [H^1(\Omega)]^3 : \mathbf{v}_{|\Gamma_D} = \mathbf{u}_S\}$ s.t.

  $$\int_\Omega [2\mu\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{v}) + \lambda \operatorname{div} \mathbf{u} \operatorname{div} \mathbf{v}]\, d\Omega = \int_\Omega \mathbf{f}^t \mathbf{v} d\Omega + \int_{\Gamma_N} \mathbf{g}_S^t \mathbf{v} d\Gamma,$$

  for all $\mathbf{v} \in [H^1_0(\Omega)]^3 = \{v \in [H^1(\Omega)]^3 : \mathbf{v}_{|\Gamma_D} = 0\}$,
  with Lamé's constants λ, μ, volume forces $\mathbf{f}$ boundary tractions $\mathbf{g}$, symmetric strains $\varepsilon(\mathbf{u})$.
- Computational domain Ω is extremely complicated, union of voxels.
- FE approximation: displacements $\mathbf{u}$ represented by piecewise trilinear polynomials.

Solving the system of equations

- System of equation
$$A\mathbf{x} = \mathbf{b}$$
A is large (huge) sparse, symmetric positive definite.
- Approach by people at ETH Inst. of Biomedical Engineering: preconditioned conjugate gradient (PCG) algorithm
  - element-by-element (EBE) matrix multiplication
  - diagonal preconditioning (Jacobi)
  - very memory economic, slow convergence as problems become large

Solving the system of equations [cont'd]

- Our new approach:
  - PCG with smoothed aggregation (SA) multilevel preconditioning

    $$AB^{-1}\mathbf{y} = \mathbf{b}, \qquad \mathbf{y} = B\mathbf{x}.$$

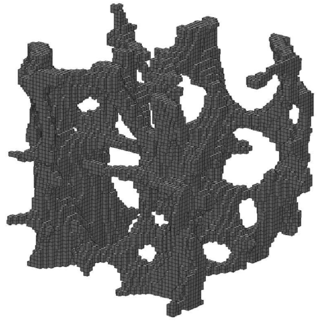
    Solving with B means applying one multigrid V-cycle.
  - Buildung the preconditioner requires forming A.
  - Parallel / scalable implementation.

Multilevel: a simple multigrid V-cycle

Approximately solve $A_\ell \mathbf{u} = \mathbf{b}$ where ℓ is the current grid level.
procedure multilevel($A_\ell, \mathbf{b}, \mathbf{u}, \ell$)
if $\ell < L$ **then**
    $\mathbf{u} = S_\ell(A_\ell, \mathbf{b}, \mathbf{u})$;
    $\hat{\mathbf{r}} = R_\ell(\mathbf{b} - A_\ell \mathbf{u})$;
    $A_{\ell+1} = R_\ell A_\ell P_\ell; \quad \mathbf{v} = \mathbf{0}$;
    multilevel($A_{\ell+1}, \hat{\mathbf{r}}, \mathbf{v}, \ell+1$); $\{A_{\ell+1} = R_\ell A_\ell P_\ell; \qquad \}$
    $\mathbf{u} = \mathbf{u} + P_\ell \mathbf{v}$;
else
    Solve $A_\ell \mathbf{u} = \mathbf{b}$;
end if

Preconditioner: Call procedure multilevel($A_0 = A, \mathbf{b}, \mathbf{u} = \mathbf{0}, L$)

Parallel mesh reading



Mesh file content

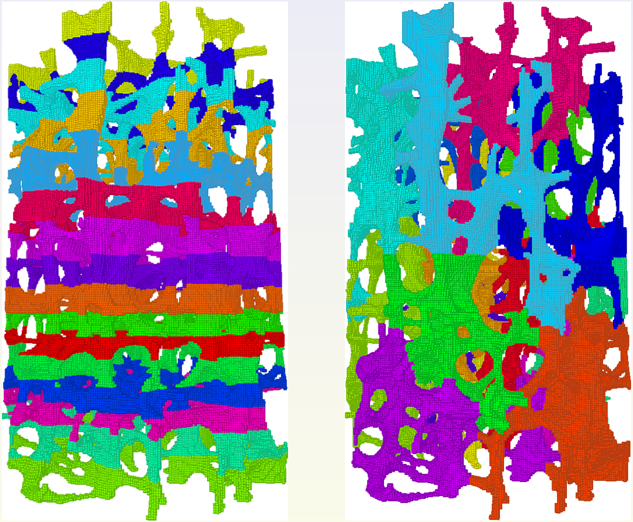
- A list of node coordinates (x, y, z)
- A list of hexahedra (8 nodes)
- A list of boundary conditions

Implementation: HDF5 format/library

- Binary file format allows for efficient I/O
- Allows for parallel I/O
- Mesh reading scales with number of processors

Mesh partitioning

- Purpose
  - Load balance: Each processor gets the same number of nodes
  - Minimize solver communication: Minimize the surface area of the interprocessor interfaces
  - Crucial for efficient parallel execution
- Implementation
  - ParMETIS: Parallel library for graph partitioning.
  - Heuristic multilevel algorithm



Initial partition (left) based on node coordinates
ParMETIS repartition (right)

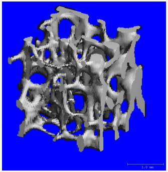
The Trilinos Software framework

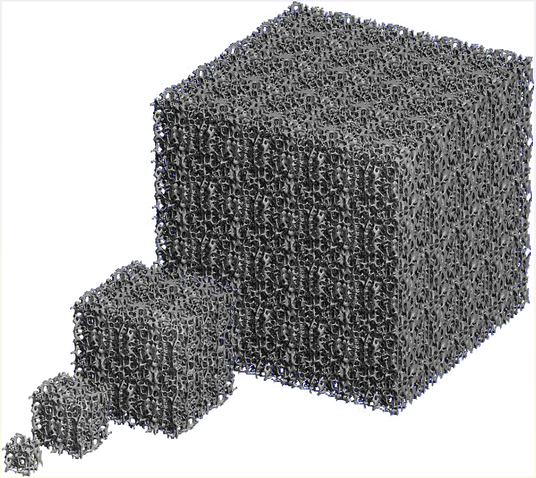
- The Trilinos Project is an effort to develop parallel solver algorithms and libraries within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific applications.
- See `http://software.sandia.gov/trilinos/`
- Provides means to distribute (multi)vectors and (sparse) matrices (Epetra package).
- Provides solvers that work on these distributed data.
- Iterative solvers and preconditioners (AztecOO/IFPACK).
- Smoothed aggregation multilevel preconditioner (ML package).
- Data distribution for parallelization (ParMETIS).
- Direct solver on coarsest level (AMESOS)

Computational environment

- Hardware: Cray XT3 (at Swiss Supercomputer Center CSCS)
  - 1100 2.6 GHz AMD Opteron processors,
  - 1 CPU with 2 GB RAM / node
  - Cray SeaStar high speed network, bandwidth 7.6 GB/s (4 GB/s sustained)
  - Peak performance is 5.9 Tflop/s.
- Software
  - UNICOS/lc, MPI-2, Trilinos (latest developers version)

Numerical experiment I: Weak Scalability test





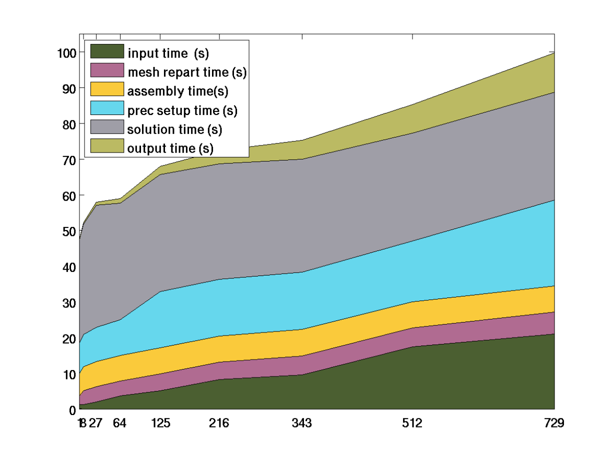
Problem size scales with the number of processors

Weak Scalability test [cont'd]

name	nodes	elements	equations
cube 1	98'381	60'482	295'143
cube 2	774'717	483'856	2'324'151
cube 3	2'609'611	1'633'014	7'828'833
cube 4	6'164'270	3'870'848	18'492'810
cube 5	12'038'629	7'560'250	36'115'887
cube 6	20'766'855	13'064'112	62'300'565
cube 7	32'983'631	20'745'326	98'950'893
cube 8	49'180'668	30'966'784	147'542'004
cube 9	70'042'813	44'091'378	210'128'439

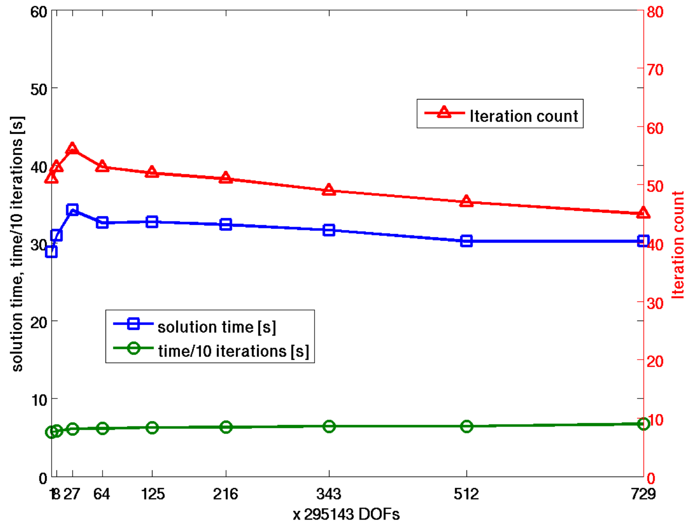
Reduction of residual error by a factor 10^5, i.e.,
$\|\mathbf{r}_k\|_2 = \|\mathbf{b} - A\mathbf{x}_k\|_2 < 10^{-5}\|\mathbf{b}\|_2$.

Weak Scalability test [cont'd]

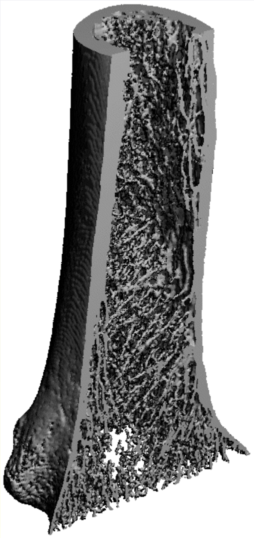


[With optimal method: execution times stay constant.]

Weak Scalability test [cont'd]



Numerical experiment II: Real world application



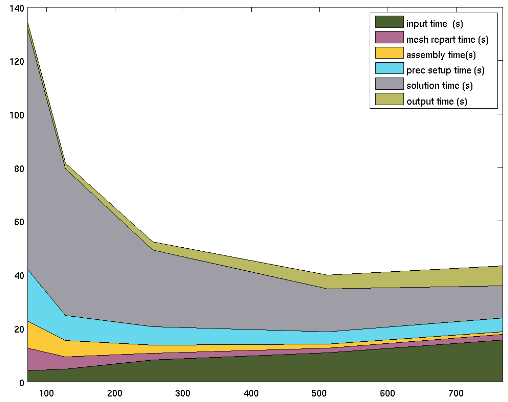
Distal part (20% of the length) of the radius in a human fore-arm.

7'761'472 nodes

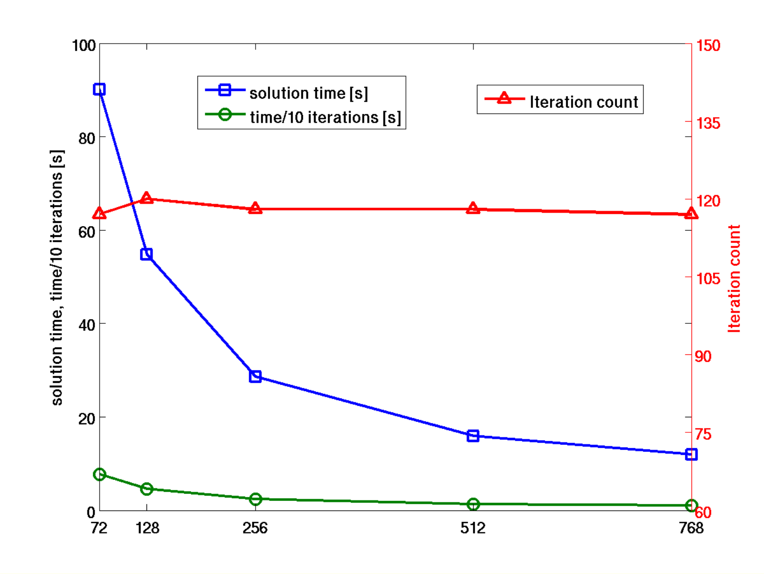
5'438'882 elements

23'284'416 degrees of freedom

Real world application [cont'd]



Real world application [cont'd]



Summary and conclusions

- Have described the model and some implementation details for multi-level μ-finite element analysis of human bone structures.
- By using the presented techniques, one can obtain a fully parallel finite element code.
- Numerical results show excellent weak and strong scalability for both an artificial model problem and a realistic human bone model.
- Future work:
  - Reduce memory consumption (again)
  - EBE approach for finest level matrix
  - Smooth surfaces / interfaces by means of *flexible hexahedral meshes*

References

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See you at:


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