Design of Finite Element Software for Modeling Bone Deformation and Failure

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Goal state

What I hope to get across today:

- Show some design choices that help make flexible FE software
  - In high-level solvers and mesh specification
  - In preconditioner construction
  - In element coding (briefly)
- Show some places where I need help from domain experts

Diagnostic toolchain

- Micro-CT (or other) scan data from patient
- Inference of material properties
- Construction of coarse FE model (voxels)
- Simulation under loading
- Output of stress fields, displacements, etc.

Software strategies

Two basic routes:

- Discretize microstructure to get giant FE model
  - Prometheus (Mark Adams) – 57M+ elements
  - ParFE (Arbenz and Sala) – 200M unknowns
- Approximate microstructure with constitutive model
  - Can do with commercial FEM codes
  - Smaller model, less compute time
  - Less detail required in input?
  - Hard to get the right constitutive model

A little history

BoneFEA started as a consulting gig

- Code for ON Diagnostics (Keaveny and Kopperdahl)
- Developed jointly with P. Papadopoulos
- Meant to replace ABAQUS in overall system
- Initial goal: some basic simulations in under half an hour
- Development work on and off 2006–2008
- More recent revisitings (trying to rebuild)

BoneFEA

- Standard displacement-based finite element code
- Elastic and plastic material models (including anisotropy and asymmetric yield surfaces)
- High-level: incremental load control loop, Newton-Krylov solvers with line search for nonlinear systems
- Library of (fairly simple) preconditioners; default is a two-level geometric multigrid preconditioner
- Input routines read ABAQUS decks (and native format)
- Output routines write requested mesh and element quantities
- Visualization routines write VTk files for use with VisIt

Basic principles

- This sort of programming seems hard (?)
  - How many man-hours went into ABAQUS?
  - Easy to lose sleep to an indexing error
- Want to reduce the *accidental* complexity
  - Express as much as possible at a high level
  - Use C++/Fortran (and libraries) for performance-critical stuff
  - Make trying new things out easy

Enabling technology

Three separate language-based tools:

- Lua-based system for loading conditions, high-level solvers
- Lua-based system for preconditioners, lower-level solver logic
- Matexpr for material model computations

In progress: solver scripting via PyTrilinos (Sandia)

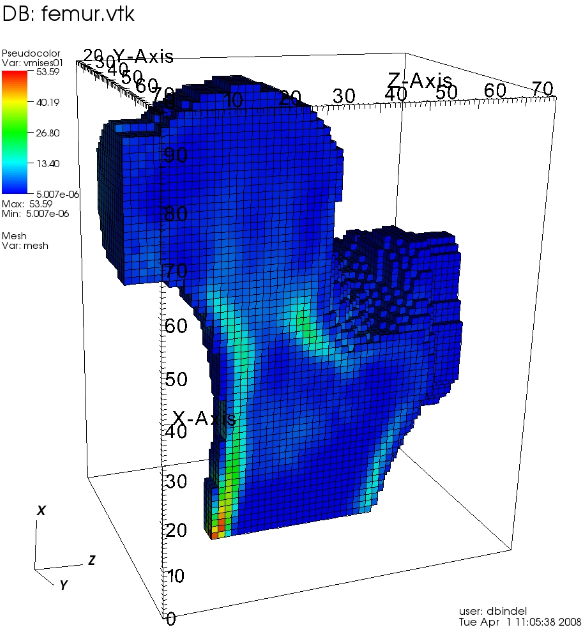
Solver quandries

A simple simulation involves *lots* of choices:

- Load stepping strategy?
- Nonlinear solver strategy?
- Linear solver strategy?
- Preconditioner?
- Subsolvers in multilevel preconditioner?

Want a simple framework for playing with options.

Example analyses



Example analysis loop

```
mesh:rigid(mesh:numnp()-1, {z='min'},
  function()
    return 'uuuuuu', 0, 0, bound_disp
  end)

pc = simple_msm_pc(mesh,20)
mesh:set_cg{M=pc, tol=1e-6, max_iter=1000}
for j=1,n do
  bound_disp = 0.2*j
  mesh:step()
  mesh:newton{max_iter=6, Rtol=1e-4}
end
```

Analysis innards

- `rigid` ties a specified part of the mesh to a rigid body (and applies boundary conditions to that rigid body)
- `step` swaps history, updates load, computes predictor
- `newton` does Newton iteration with line search; specify
  - Max iterations
  - Residual tolerance
  - Line search parameters (Armijo constant α)
  - What linear solver to use
  - Whether to update the preconditioner
- Also have `mnewton` (modified Newton)

Preconditioning

- Accelerate iterative solver with *preconditioner*
- Often built from simpler blocks
  - Basic iterative solver passes
  - Block solves
  - Coarse grid solves
- Want a simple way to assemble these blocks

Preconditioner specification (library code)

```
function simple_msm_pc(mesh, ncgrid, nsmooth, omega)
  local pcc = form_coarse_pc2(mesh, ncgrid)
  local pc  = {}
  local K   = mesh.K
  nsmooth = nsmooth or 1
  function pc:solve(x,b) ... end
  function pc:update() pcc:update() end
  function pc:delete() ... end
  return pc
end
```

Preconditioner specification (library code)

```
function pc:solve(x,b)
  self.r  = self.r  or QArray:new(x:m(),1)
  self.dx = self.dx or QArray:new(x:m(),1)

  mesh_bgs(mesh.mesh,mesh.K,x,b,nsmooth)
  K:apply(x,self.r)
  self.r:sub(b)

  pcc:solve(self.dx,self.r)
  x:sub(self.dx)
  K:apply(x,self.r)
  self.r:sub(b)

  mesh_bgs(mesh.mesh,mesh.K,self.dx,self.r,nsmooth)
  x:sub(self.dx)
end
```

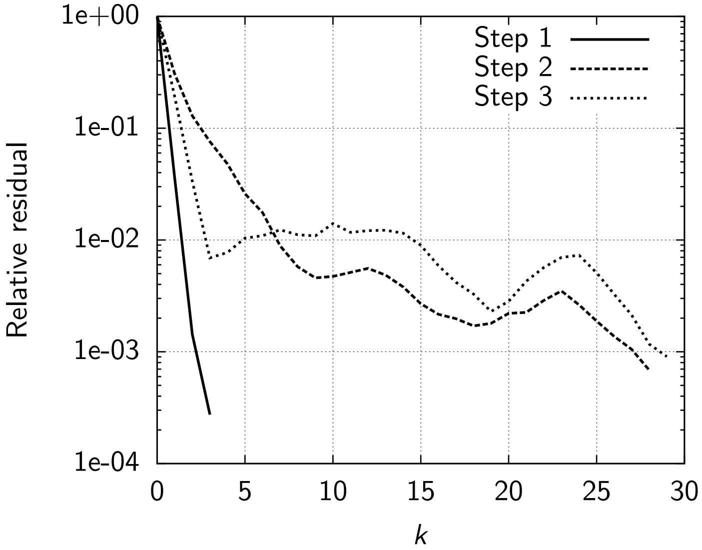
The problem of preconditioning

Standard preconditioners work best for

- Simple geometries
- Constant or smoothly varying coefficients
- Isotropic materials
- Strongly definite problems

Macroscopically, bone breaks almost all of these!

Preconditioning triumphs and failures



Preconditioning triumphs and failures

- We do pretty well with two-level geometric multigrid
  - 18 steps, 15 s to solve femur model on my laptop
- ... up until plasticity starts to kick in
- Needed: a better (physics-based) preconditioner
- Usual key: physical insight into macroscopic behavior

Material modeling

BoneFEA provides general plastic element framework; specific material model provided by an object. Built-in:

- Isotropic elastic
- Orthotropic elastic
- Simple plastic
- Anisotropic elastic / isotropic plastic
- Isotropic elastic / asymmetric plastic yield surface

How do we make it simplify to code more?

Partial solution: Matexpr

- Relatively straightforward in MATLAB – but slow
- Use Matexpr to translate MATLAB-like code to C
- Supports basic matrix expressions, symbolic differentiation, function definitions.
- Takes advantage of symmetry, sparsity, redundancy to optimize generated code
- Does not provide control flow (that's left to C)

Matexpr in action

Extract the deviatoric part of the elastic constitutive tensor:

```
void ME::compute_Cd(double* Cd)
{
    /* <generator matexpr>
    input symmetric DGelastic(9,9);
    output Cd(9,9);
    m  = [1; 1; 1; 0; 0; 0; 0; 0; 0];
    Iv = m*m'/3.0;
    Id = eye(9) - Iv;
    Cd = Id*DGelastic*Id;
    */
}
```

Conclusion

- Initial BoneFEA work for ON Diagnostics is done.
- Currently re-implementing similar functionality in an open package (as part of a more general framework).
- Problems and physical insights both welcome!