CS/CNS 257c: Simulation
Due Friday, April 30: *written submission* 4:00pm, *electronic submission* 11:59pm

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# Homework 3

1. **Implement the PBCG algorithm.**

   We discussed in class the BCG (bi-conjugate gradient) algorithm. In this homework you are asked to implement the preconditioned version of this algorithm, PBCG. Recall the BCG requires symmetry exclusive or positive-definiteness. For systems which are symmetric (or positive-definite) various quantities will be identical. Ideally you should setup your implementation in such a way that you can take advantage of these simplifications when they apply. For purposes of notation we consider the system $Ax = b$. Your variables $x$ will be displacements. Additionally you will need storage for two residual vectors $\bar{r}$ and $r$ as well as the directions $\bar{p}$ and $p$. To deal with preconditioning you will also need $\bar{z}$ and $z$. The preconditioner will be denoted by $B$.

   The algorithm is initialized by computing

$$\begin{aligned} x_0 &= 0 \\ \bar{p}_0 &= p_0 = \bar{r}_0 = r_0 = b - Ax_0 \\ z_0 &= Br_0 \\ \bar{z}_0 &= B^T \bar{r}_0. \end{aligned}$$

   Once we do dynamics you may find it advantageous to initialize $x_0$ to the solution of the previous step. Then run until convergence

$$\begin{aligned} \alpha_k &= \frac{\bar{r}_k^T z_k}{\bar{p}_k^T A p_k} \\ x_{k+1} &= x_k + \alpha_k p_k \\ r_{k+1} &= r_k - \alpha_k A p_k \\ \bar{r}_{k+1} &= \bar{r}_k - \alpha_k A^T \bar{p}_k \\ z_{k+1} &= Br_k \\ \bar{z}_{k+1} &= B^T \bar{r}_k \\ \beta_k &= \frac{\bar{r}_{k+1}^T z_{k+1}}{\bar{r}_k^T z_k} \\ p_{k+1} &= z_{k+1} + \beta_k p_k \\ \bar{p}_{k+1} &= \bar{z}_{k+1} + \beta_k \bar{p}_k. \end{aligned}$$

   The simplest choice (and only choice for now) is to use a diagonal preconditioner, i.e., the action of $B$ divides each row by the diagonal element of $A$.

The above version will work for non-symmetric but positive definite $A$. If $A$ is in addition symmetric $\bar{p}_k = p_k$, $\bar{r}_k = r_k$, and $\bar{z}_k = z_k$ for all $k$, cutting your work in half. If $A$ is symmetric but not positive definite, set $\bar{r}_k = Ar_k$ and $\bar{p}_k = Ap_k$ for all $k$. (If it is neither you have to use a more general method such as GMRES). Note however that if you happen to have a good preconditioner you might as well run the ordinary conjugate gradient algorithm on the problem $A^T Ax = A^T b$.

As a stopping criterion use the size of the relative residual, i.e., iterate until it is smaller than some chosen threshold

$$\frac{\|B(Ax - b)\|}{\|Bb\|} < \epsilon.$$

For your implementation you will, in particular, need to compute $Av$ and $A^T v$ for various vectors $v$. For this to be efficient you can either assemble your matrix into some sparse form, or leave it unassembled. The latter is recommended, though sometimes it is just as easy to make a sparse version of the assembled matrix.

Verify your implementation by using some test problems for which you know the answer and also ask MATLAB for its answer.

2. **Time integration.**

   Consider the homogeneous scalar model equation

$$\dot{u} - au = 0$$

   for the investigation of the stability of the backward, forward and trapezoidal integration methods. For each method compute the polynomial $\rho(z)$. Sketch the root of the polynomial with respect to $a\Delta t$ in the complex plane, where $\Delta t$ is the time step size. In what range should the time step size be chosen with respect to the stiffness term $a$ for practical computations?

3. **Truss structure revisited.**

   (a) Implement the consistent and lumped mass matrices in your finite element program from the previous homework. For the time integration of the second order semi-discrete initial value problem, implement a generalized Newmark scheme.

   (b) For the numerical investigation of the truss structure of the previous homework, we choose as initial conditions a displacement of $u = 0.2$ and velocity $\dot{u} = 0$ at the top of the structure. The initial displacements and velocities at the remaining nodes are zero. We choose the material density to be 20.

   Compute the structure with implicit ($\beta = 0.25$, $\gamma = 0.5$) and explicit ($\beta = 0$, $\gamma = 0.5$) time integration. The time step size of the implicit scheme should be 10, 100 and 1000 times the critical time step size for the explicit scheme.

Visualize and compare the time evolution of the displacements of the structure top. Compare the approximate computation times for both methods.