POD acceleration of fully implicit solver for unsteady non-linear flows and its application on grid architecture

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1. Motivations

We propose in this paper a technique to accelerate the convergence of the Newton method to solve non-linear unsteady CFD problems. The principle relies on an effective way to obtain a better solution for the current time step than the solution of the previous time step. This is performed on a reduced model computed with a Proper Orthogonal Decomposition of some solution computed at some previous time step. The developed methodology fits the grid computing design with a client server approach to compute the POD components necessary for the acceleration. We will shows on several flows configurations the effective computational saving obtained with the proposed technique.

Let us recall briefly the fully implicit discretizations of unsteady nonlinear problems. Let $L(u)$ be a nonlinear discrete operator representing a spatial approximation of a parabolic boundary value problem. The simplest robust technique for time approximation of unsteady problems is the backward Euler time stepping:

$$\frac{u^i - u^{i-1}}{\Delta t} + L(u^i) = g^i.$$ \hspace{1cm} (1)

The main advantage of the method is its unconditional stability. Being the first order scheme (in time), it may be generalized to the higher order approximations (e.g., BDF time stepping). In general, the $i$th time step of a fully implicit scheme may be represented by the nonlinear system $F^i(u^i) = 0$, where $F^i$ contains all the problem data and previous solutions. For instance, in the case of scheme (1),

$$F^i(u^i) = u^i + L(u^i)\Delta t - u^{i-1} - g^i\Delta t.$$ \hspace{1cm} (2)

The price to be paid for the robustness of the method is its arithmetical complexity: at each time step, a nonlinear system has to be solved. In last decade, several robust

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nonlinear solvers have been proposed, analyzed, and implemented ([4] p. 303). However, the efficient solution of large nonlinear systems remains a challenge.

The inexact Newton backtracking [5,4,2] method offers global convergence properties combined with potentially fast local convergence. Algorithm INB presumes the choice of initial guesses \( u_k \) for nonlinear iterations. We recall that the arithmetical complexity of the method is expressed in the total number of function evaluations \( n_{evF} \) and total number of preconditioner evaluations \( n_{evP} \) (if any), the remaining overheads are negligible.

2. Initial guess for the Newton solution with POD

Proper orthogonal decomposition (POD) provides a way to find optimal lower dimensional approximations of the given series of data. More precisely, it produces an orthonormal basis for representing the data series in a certain least squares optimal sense [1]. Combined with the Galerkin projection, POD is a tool for generation of reduced models of lower dimension. The reduced models may give a better initial guess for the Newton solution at the next time step.

POD provides the definite answer to the question: What \( m \)-dimensional subspace \( S \subset \mathbb{R}^N \) is the most close (in the terms of the least squares) to the given set of vectors \( \{u^i\}_{i=1}^n \)?

Here \( P_S \) is the orthogonal projection onto \( S \). Define the correlation matrix \( R = XX^T \), \( X = \{u^1 \ldots u^n\} \), and find \( m \) eigenvectors of the problem

\[
R w_j = \lambda_j w_j, \quad \lambda_1 \geq \ldots \geq \lambda_N \geq 0
\]
corresponding to \( m \) largest eigenvalues \( \lambda_1 \geq \ldots \geq \lambda_m \). Then \( S = \text{span}\{w^j\}_{j=1}^m \) and

\[
\sum_{i=1}^n \|u^i - P_S u^i\|^2 = \sum_{j=m+1}^N \lambda_j.
\]

Computational cost of finding \( m \)-largest eigenvalues of symmetric matrix \( R \) is not high. Indeed, our experience shows that for \( m = O(10) \) the application of the Arnoldi process requires a few tens of \( R \)-matrix-vector multiplications in order to retrieve the desirable vectors with very high accuracy [3]. In spite of large dimension \( N \) and density of \( R \), the matrix-vector multiplication is easy to evaluate, due to the factored representation \( R = XX^T \). The arithmetical cost of the evaluation \( Xa \) (and \( X^Tb \)) is \( Nn \) multiplications and not more than \( Nn \) additions, therefore, \( R \)-matrix-vector multiplication costs at most \( 4Nn \) flops.

Each time step of the scheme (1) generates the equation (2) which we call the original model. A reduced model is generated on the basis of POD for a sequence of solutions at time steps \( \{u^i\}_{i=i_b}^{i_e}, \quad i_e - i_b + 1 = n \). The eigenvectors \( \{w^j\}_{j=1}^m \) may be considered as the basis of \( m \)-dimensional subspace \( V_m \subset \mathbb{R}^N \). The reduced model is the Galerkin projection onto this subspace: \( V_m^T F^i(V_m \hat{u}^i) = 0 \), or, equivalently with \( \hat{u}^i \in \mathbb{R}^m \) and \( \hat{F}^i : \mathbb{R}^m \to \mathbb{R}^m : \hat{F}^i(\hat{u}^i) = 0 \),
The reduced model is the nonlinear equation of very low dimension $m$. For its solution, we adopt the same INB algorithm with finite difference approximation of Jacobian-vector multiplication. Being the formal Galerkin projection, each evaluation of function $\hat{F}_i(\hat{u}_i)$ is the sequence of the following operations:

$$u_i = V_m \hat{u}_i, f_k = F_i(u_k), f_i = V_m^T f_k.$$ Therefore, the overhead is matrix-vector multiplications for $V_m$ and $V_m^T$, i.e., $4Nm$ flops. We notice that usually $m = O(10)$ and the evaluation of function $F(u)$ is much more expensive than $40Nm$ which implies a negligible weight of the overheads. Another important consequence of low dimensionality of (4) is that INB algorithm may be applied without any preconditioner.

### 2.1. Fully implicit solver with POD-reduced model acceleration

Coupling POD and Galerkin projection for the generation of the reduced model gives a powerful tool for acceleration of the fully implicit schemes. Let $n$, the length of data series be defined, as well as the desirable accuracy $\epsilon$, for $F_i()$: $\|F_i(u^i)\| \leq \epsilon$. For any time step $i = 1, \ldots$, perform:

**Algorithm**

**IF** $i \leq n$, **SOLVE** $F_i(u^i) = 0$ **BY** PRECONDITIONED INB **WITH** THE INITIAL GUESS $u_0^i = u^{i-1}$ **AND** ACCURACY $\epsilon$

**ELSE**

1. **IF** $(mod(i, n) = 1)$:

   (a) **FORM** $X = \{u_{i-n}, \ldots, u_{i-1}\}$;

   (b) **FIND** SO MANY LARGEST EIGENVECTORS $w_j$ OF $R = XX^T$ THAT $\sum_{j=m+1}^{N} \lambda_j \leq \epsilon$;

   (c) **FORM** $V_m = \{w_1, \ldots, w_m\}$

2. **SET** $\hat{u}_0 = V_m^T u_{i-1}$

3. **SOLVE** $\hat{F}_i(\hat{u}^i) = 0$ **BY** NON-PRECONDITIONED INB **WITH** THE INITIAL GUESS $\hat{u}_0^i$ **AND** ACCURACY $\epsilon/10$

4. **SET** $u_0^i = V_m \hat{u}^i$

5. **SOLVE** $F_i(u^i) = 0$ **BY** PRECONDITIONED INB **WITH** THE INITIAL GUESS $u_0^i$ **AND** ACCURACY $\epsilon$

Several remarks are in order. The absence of the preconditioner for the reduced model is dictated by two reasons: a) it is not clear how to construct a preconditioner for the reduced model, b) it is hardly needed if $m$ is small. The reduced model is slightly oversolved: this provides better initial guess $u_0^i$. The number of eigenvectors is chosen adaptively in the above algorithm: it allows to form such a reduced model that approximate the original model with the desirable accuracy $\epsilon$. Actually, this condition my be replaced by a more rough $N\lambda_{m+1} < \epsilon$ or even a fixed number $m$, $m = 10 - 40$. Solution of the eigenvalue problem may be performed asynchronously with the implicit solution: as soon as $V_m$ is formed, the reduced model becomes the active substep. The latter observation allows
Table 1

<table>
<thead>
<tr>
<th></th>
<th>without POD</th>
<th>with POD $m=10$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i$</td>
<td>10 20 30</td>
<td>40 50 60 70 80</td>
</tr>
<tr>
<td>$u_i = u_i^{i-1}$</td>
<td></td>
<td>$u_i = V_m u_i$</td>
</tr>
<tr>
<td>$|F(u_i^0)|$</td>
<td>0.3 0.8 0.1</td>
<td>8 $\cdot$ 10^{-6} 10^{-5} 10^{-6} 3 $\cdot$ 10^{-6} 10^{-6}</td>
</tr>
<tr>
<td>$n_{evF}$</td>
<td>193 184 173</td>
<td>42+39 43+36 46+11 46+21 36+12</td>
</tr>
<tr>
<td>$n_{precF}$</td>
<td>187 178 167</td>
<td>0 +36 0 +32 0 + 9 0 +18 0 +10</td>
</tr>
<tr>
<td>time</td>
<td>16 15 15</td>
<td>0.9+3.1 1+2.6 1+0.7 1+1.4 0.8+0.8</td>
</tr>
<tr>
<td>full model</td>
<td>Reduced model + full model</td>
<td></td>
</tr>
</tbody>
</table>

Effect of POD acceleration for the lid driven cavity 2D problem modelled by the biharmonic streamfunction equation with a periodic drive.

We will investigate the powerful of the proposed approach on the lid driven cavity flows where the boundary conditions give three set of solutions: transient to a steady flow, quasi-periodic flow, periodic flow with variable (arrhythmic) periods.

Table 1 shows that the initial function value drops from $10^{-1}$ without POD acceleration to $10^{-6}$ with. The elapsed time is then reduced by a factor 6 on a alpha ev67 processor. The mesh size is $h = 256^{-1}$ leading to 65025 dof, the stopping criterion for INB is $\|F_i^0(u_i^0)\| < 10^{-7}\|F^0(0)\|$. The time step is $\Delta t = 5$ leading to have 13 time steps per period and $m = 10$. $V_m$ are produced starting from 20th step.

REFERENCES