ACCELERATION OF IMPLICIT SCHEMES USING REDUCED MODELS AND GRID COMPUTING

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Instead of introduction

movie

Complexity and parallelization

- OpenMP computation of droplet

  1100 time steps, $h = 8^{-1} - 512^{-1}$, no parallel solvers

# cores Intel Xeon 2.6 Ghz	2	4	8
Time, hours	30.50	22.84	18.815

- MPI visualization of flooding

  Povray-MPI, resolution 4096×3072 of single frame

# cores Intel Xeon 2.6 Ghz	15	30	60	120
Time, seconds	367	195	107	62

- Parallel computing technology should correspond to algorithm
- I proceed to an algorithm which fits to GRID computing

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Acceleration of implicit schemes using reduced models and grid computing

Joint work with

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D.Tromeur-Dervout, Yu.V., Journal of Computational Physics, 219, 2006

D.Tromeur-Dervout, Yu.V., Advances in Engineering Software, 38, 2007

Inexact Newton backtracking method for $F(u) = 0$

S.Eisenstat, H.Walker,'90s

- Newton: $F'(u_k)s_k = -F(u_k)$, $u_{k+1} = u_k + s_k$

- Inexact Newton: $\|F(u_k) + F'(u_k)s_k\| \leq \eta_k \|F(u_k)\|$
  $\eta_k = |\|F(u_k)\| - \|F(u_{k-1}) + F'(u_{k-1})s_{k-1}\||/\|F(u_{k-1})\|$

- Inexact Newton Backtracking:
  while $\|F(u_k + s_k)\| > [1 - 10^{-4}(1 - \eta_k)]\|F(u_k)\|$
  update $s_k \leftarrow \theta s_k$ and $\eta_k \leftarrow 1 - \theta(1 - \eta_k)$
  $u_{k+1} = u_k + s_k$

$F'(u_k)v = \frac{1}{\delta}[F(u_k + \delta v) - F(u_k)]$

NITSOL H.Walker,'98

Fully implicit schemes

Backward Euler: $\frac{u^i - u^{i-1}}{\Delta t} + A(u^i) = g^i$, or

$$F^i(u^i) = 0$$

For $i = 1, \ldots$:

- set $u_0^i = u^{i-1}$
- solve $F^i(u^i) = 0$ by INB

Idea: get better u_0^i by POD and Reduced Model

Related works

- P.Fischer '98, M.Clemens et al.'03 — reconstruction from $u^{i-m}, \ldots, u^{i-1}$
- M.Rathinam, L.Petzold '03 — review of POD and RM
- D.Tromeur-Dervout, Yu.V. '05,'06,'07 — INB+POD+RM
- R.Marcovinovic, J.Jansen '07 — POD-RM for linear schemes

Proper orthogonal decomposition

What vector $v \in R^N$ is the most close to $\{u^i\}_{i=1}^n$:

$$v = \arg\min_{v \in R^N} \sum_{i=1}^{n} \|u^i - P_v u^i\|^2?$$

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$$v = \arg \min_{v \in R^N} \sum_{i=1}^{n} \|u^i - P_v u^i\|^2 ?$$

Generate correlation matrix $R = XX^T$, $X = \{u^i\}$

$$Rw_j = \lambda_j w_j, \quad \lambda_1 \geq \cdots \geq \lambda_N \geq 0$$

$$v = w_1 \;\rightarrow\; \sum_{i=1}^{n} \|u^i - P_v u^i\|^2 = \sum_{j=2}^{N} \lambda_j$$

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or generate $n \times n$-matrix $r = X^T X$, $X = \{u^i\}$

$$r\hat{w}_j = \mu_j \hat{w}_j, \quad \mu_1 \geq \cdots \geq \hat{\mu}_n \geq 0$$

$$\lambda_j = \mu_j, \quad w_j = X\hat{w}_j, \quad j = 1, \ldots, n$$

Proper orthogonal decomposition

What m-dimensional subspace S is the most close to $\{u^i\}_{i=1}^n$?

$$S = \mathrm{span}\{w_j\}_{j=1}^m \;\to\; \sum_{i=1}^{n} \|u^i - P_S u^i\|^2 = \sum_{j=m+1}^{N} \lambda_j$$

How to use POD?

- Given $u^1, ..., u^n$ and small integer m
- Form $X = \{u^1, ..., u^n\}$, $R = XX^T$ (or $r = X^T X$)
- Find m largest e.-v. of $Rw_j = \lambda_j w_j$, $(w_i, w_j) = \delta_{ij}$
- Form Reduced Model basis $V_m = \{w_1, ..., w_m\}$
- Form Reduced Model problem $V_m^T F(V_m \hat{u}) = 0$

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problem $V_m^T F(V_m \hat{u}) = 0$ has low dimension!

How to use Reduced Model?

- Solve Reduced Model problem $\hat{F}(\hat{u}) = V_m^T F(V_m \hat{u}) = 0$ by INB
- Project the solution to R^N: $u_0 = V_m \hat{u}$
- Use u_0 as initial guess for $F(u) = 0$

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INB for $\hat{F}(\hat{u}) = 0$:

- Evaluation of $\hat{F}$ requires $V_m \cdot$, $F(\cdot)$, $V_m^T \cdot$
- No preconditioning (small m)

Fully implicit schemes accelerated by POD and RM

Choose n, $\epsilon > 0$. For $i = 1, ...$

If $i \leq n$ solve $F^i(u^i) = 0$ with accuracy ϵ and $u^i_0 = u^{i-1}$

Fully implicit schemes accelerated by POD and RM

Choose n, $\epsilon > 0$. For $i = 1, \ldots$

If $i \le n$ solve $F^i(u^i) = 0$ with accuracy ϵ and $u_0^i = u^{i-1}$

Else

1. if($mod(i,n) = 1$): form $X = \{u^j\}_{j=i-n}^{i-1}$, $R = XX^T$,

   form RM basis $V_m = \{w_j\}_{j=1}^{m}$: $\sum\limits_{k=m+1}^{N} \lambda_k < \epsilon$
2. solve $V_m^T F^i(V_m \hat{u}^i) = 0$ with accuracy $\epsilon/10$ ←Reduced Model
3. set $u_0^i = V_m \hat{u}^i$ ←Initial Guess
4. solve $F^i(u^i) = 0$ with accuracy ϵ ←Original Model

step 1 produces the reduced model basis (seldom)

step 2 solves implicitly the reduced model without preconditioning (m is small)

step 3 gives better initial guess for the original problem to be solved at step 4

adaptive choice of m may be replaced by $N\lambda_{m+1} < \epsilon$, or even fixed m

Example: unsteady lid driven cavity (2d NS)

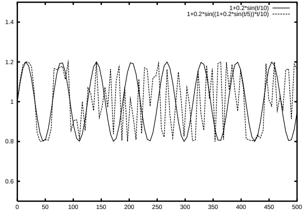
Streamfunction formulation

$$-\frac{\partial}{\partial t}(\Delta\psi) + \frac{1}{Re}\Delta^2\psi + (\psi_y(\Delta\psi)_x - \psi_x(\Delta\psi)_y) = 0$$

$$\psi = 0 \text{ on } \partial\Omega, \ \frac{\partial\psi}{\partial n} = \begin{cases} v(t) & \text{if } y = 1 \\ 0 & \text{if } 0 \le y < 1 \end{cases}$$

$\psi|_{t=0} = 0 \quad v(t) = 1 + 0.2\sin(t/10) \rightarrow$ quasi-periodic

$\psi|_{t=0} = 0 \quad v(t) = 1 + 0.2\sin([1 + 0.2\sin(t/5)]t/10) \rightarrow$ arrhythmic flow



GMRES preconditioned by $\frac{1}{Re}\Delta^2 \rightarrow$ independence of mesh size for $Re = 10^3$

Effect of POD-RM for quasi-periodic case

$h = 256^{-1} \to$ 65025 dof, $\|F^i(u_k^i)\| < 10^{-7}\|F^0(0)\|$
$\Delta t = 5 \to\sim 13$ time steps per period

$n = 20 \to X = \{u^{20k-10} \dots u^{20k+9}\},\ k = 1, 2, \dots$
dimension of the reduced model $m = 10$.

$m = 10$ eigenvectors is more than enough: $\lambda_1 = 4.7 \cdot 10^3$, $\lambda_{10} = 5.6 \cdot 10^{-8}$

Arnoldi process with 50 multiplications by matrix $R \to$

$$\|Rw_1 - \lambda_1 w_1\|/\lambda_1 = 5 \cdot 10^{-16},\ \|Rw_{10} - \lambda_{10} w_{10}\|/\lambda_{10} = 8 \cdot 10^{-7}$$

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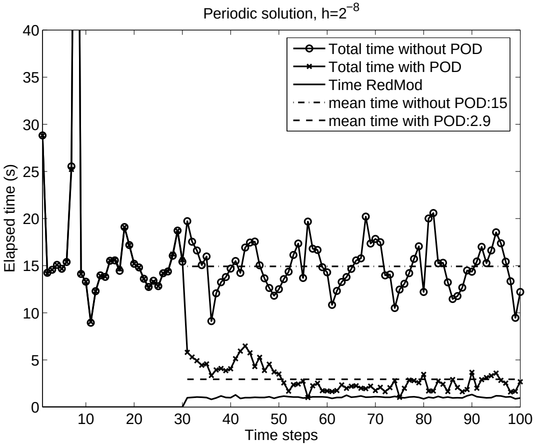

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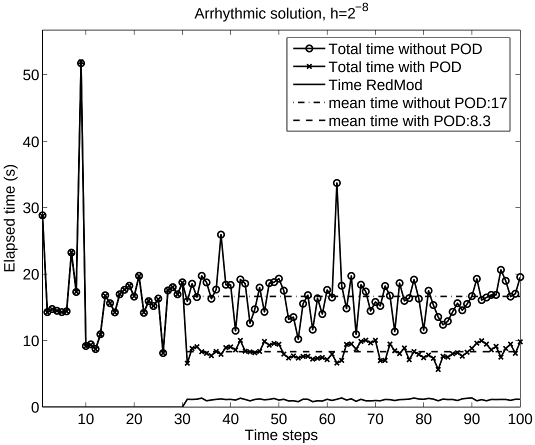
i	10	20	30	32	52	72
	$u_0^i = u^{i-1}$			$u_0^i = V_m \hat{u}^i$		
$\Vert F(u_0^i)\Vert$	0.36	0.79	0.09	$22 \cdot 10^{-6}$	10^{-6}	$2.6 \cdot 10^{-6}$
n_{evF}	166	186	189	44+55	45+11	44+19
n_{precF}	160	180	183	0+51	0+ 9	0+16
CPU	13.4	15.3	16.1	1.2+4.2	1.1+1.1	1.1+1.2

average acceleration 5-6 times

Effect of POD-RM for arrhythmic case



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i	10	20	30	32	52	72
	$u_0^i = u^{i-1}$			$u_0^i = V_m \hat{u}^i$		
$\lVert F(u_0^i)\rVert$	0.01	2.2	1.3	$5 \cdot 10^{-4}$	$4 \cdot 10^{-4}$	$2 \cdot 10^{-4}$
n_{evF}	115	205	227	50+98	42+80	49+77
n_{precF}	110	198	221	0+93	0+75	0+72
CPU	9.2	16.7	19.5	1.3+7.7	1.0+6.4	1.1+5.9

average acceleration 2 times

GRID application

Architecture of application

Two types of remoted computing resources:

Solver $\longleftrightarrow$ **PODgenerator**

Features of GRID architecture and POD acceleration

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  - no idling due to asynchronous non blocking communications

$$POD(generator) \leftrightarrow Solver$$

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    It can spawn a new set of MPI processes on Solver resource

    It can provide last solution recovered from the reduced model (no backup)

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- POD resource may work with several tasks
  - Its task is waiting data from Solver and computing POD basis
  - Due to asynchronous non blocking communications it can
    - serve other Solvers
    - make post-processing (visualization, a posteriori error estimates)

Example: unsteady driven cavity (2d NS)

A Computer A = SGI Altix350

(2 Ithanium 1.3Ghz/3Mo, 1.3Gb/s network bandwidth)

B Computer B = Linux cluster

(AMD BiAthlon 1600+ MP, 100Mb/s network bandwidth)

N Network = latency 140 μs, maximum bandwidth $71 Mb/s$

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Solver resource = Computer A
POD resource = Computer B

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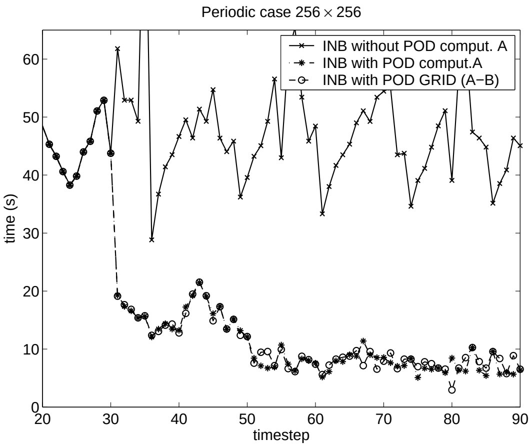

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