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Lecture: Decomposition Methods

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Outline of the talk

- 0) Motivation of Decomposition methods
- 1) Ideas for Consistency and Stability Results of Iterative Operator Splitting Methods
- 2) Numerical Results

Introduction

Decomposition methods are a powerful method of numerical investigation of complex (physical) time-dependent models, where the stationary part (elliptic) consists of simpler operators, e.g. :

- 1 Transport-Reaction Processes, see [Hundsdoerfer, Verwer 2003]
- 2 Hamiltonian Systems, see [McLachlan94], [Hairer, Lubich, Wanner 02]
- 3 Air pollutant models, see [Zlatev95]
- 4 Wave propagation models, see [Roger et al 1999]
- 5 Maxwell equations, see [Horvath06]

Introduction

Decomposition Methods

- Time- and Spatial-decomposition methods:

Contribution with the decomposition

- Decoupling the time-scales, space-scales. (Idea: Reduction of stiffness by decoupling into simple non-stiff operators).
- Decoupling the multi-physics. (Idea: Reduction of unphysical behaviours with best choice of discretization and solver methods)
- Time- and Space-adaptivity. (Idea: Efficient and accurate computations)
- Parallelization in Time and Space. (Idea: Reduction of computational time)

Motivation: Efficient and fast algorithms with sufficient accuracy and simple implementations.

Splitting Idea (Sequential Splitting)

We decouple a differential equation

$$\begin{aligned} \frac{\partial c(x, t)}{\partial t} &= \Delta c - \mathbf{v} \nabla c, (x, t) \in \Omega \times [0, T] & (1) \\ c(x, 0) &= c_0(x) \quad x \in \Omega, \quad c(x, t) = 0, (x, t) \in \partial\Omega \times [0, T], \end{aligned}$$

into two simpler parts:

$$\frac{\partial c_1(x, t)}{\partial t} = \Delta c_1, (x, t) \in \Omega \times [0, T] \quad (2)$$

$$c_1(x, 0) = c_0(x) \quad x \in \Omega, \quad c_1(x, t) = 0, (x, t) \in \partial\Omega \times [0, T]$$

$$\frac{\partial c_2(x, t)}{\partial t} = -\mathbf{v} \cdot \nabla c_2, (x, t) \in \Omega \times [0, T] \quad (3)$$

$$c_2(x, 0) = c_1(x, t) \quad x \in \Omega, \quad c_2(x, t) = 0, (x, t) \in \partial\Omega \times [0, T],$$

Splitting Idea (In general)

- 1.) Searching splitting methods, which conserves the physical behaviours (e.g. Symplectic Splitting, Flux splitting).
- 2.) Searching splitting methods with high accuracy, e.g. higher order schemes.
- 3.) Searching a "best" decomposition for operators in the splitting methods, e.g. eigenvalues of the operators to obtain their scales.
- 4.) Leave all operators in the splitting scheme to respect their influence in the solution.

Benefits of Iterative Splitting Methods

The traditional splitting methods (non-iterative) may have some drawbacks:

- for non-commuting operators we may have a very large constant in the local splitting error which requires the use of unrealistically small splitting time step;
- within a full splitting step in one sub-interval the inner values aren't approximate to the solution of the original problem;
- splitting the original problem into the different sub-problems with one operator (i.e. neglect the other components) is physically questionable.

To avoid such problems we leave all operators in the schemes and solve a fix-point problem which iterates over each operators in the inhomogeneous differential equations.

Iterative Operator Splitting Methods

$$\frac{\partial c_i(t)}{\partial t} = A c_i(t) + B c_{i-1}(t), \text{ with } c_i(t^n) = u^n, \quad (4)$$

$$\frac{\partial c_{i+1}(t)}{\partial t} = A c_i(t) + B c_{i+1}(t), \text{ with } c_{i+1}(t^n) = u^n, \quad (5)$$

where $c_0(t)$ is any fixed function for each iteration. (Here, as before, u^n denotes the known split approximation at the time level $t = t^n$.) The split approximation at the time-level $t = t^{n+1}$ is defined as $c_{\text{sp}}^{n+1} = c_{2m+1}(t^{n+1})$.

Error of the iterative method for bounded operators

Theorem

The error for the splitting methods is given as :

$$\|e_i\| = K\|B\|\tau\|e_{i-1}\| + O(\tau^2) \quad (6)$$

and hence

$$\|e_{2m+1}\| = K_m\|e_0\|\tau^{2m} + O(\tau^{2m+1}), \quad (7)$$

where τ is the time-step, e_0 the initial error $e_0(t) = c(t) - c_0(t)$ and m the number of iteration-steps, K and K_m are constants, $\|B\|$ is the maximum norm of operator B . A and B are bounded, monotone operators, e.g. from a ODE system.

Proof : Taylor-expansion and estimation of exp-functions. See the work [Geiser+Farago, 2005].

Error of the iterative method for unbounded operators

Problem for the unbounded operators in the differential formulation, we may lose smoothness in the differential formulation, see:

$$\frac{\partial c_1}{\partial t} = A c_1 + B c_0, c_1 \in C^k(H^s(\Omega) \times [0, T]), \quad (8)$$

$$\frac{\partial c_2}{\partial t} = A c_1 + B c_2, c_2 \in C^k(H^{s-2}(\Omega) \times [0, T]), \quad (9)$$

$$\frac{\partial c_3}{\partial t} = A c_3 + B c_2, c_3 \in C^k(H^{s-1}(\Omega) \times [0, T]), \quad (10)$$

where $A = \nabla D \nabla$ and $B = -\mathbf{v} \cdot \nabla$.

Solution : Integral formulation with variation of constants to bound the operators and stabilisation with full time-space discretization to balance the regularity.

Error of the iterative method for unbounded operators

Integral-Formulation and extension of the exp-operator, e.g. with variation of constants:

$$\begin{aligned} \exp((A + B)\tau)c_n &= \exp(A\tau) & (11) \\ + \int_{t^n}^{t^{n+1}} \exp(As)B \exp((t^{n+1} - s)(A + B))u_n ds \end{aligned}$$

Ideas, see [Jahnke+Lubich, 1999], [Ostermann+Hansen, 2007]
 The estimations of an unbounded operator:

$$\|A^\alpha \exp(A\tau)\| \leq \kappa\tau^{-\alpha} \quad (12)$$

$$\|A^\alpha \exp((A + B)\tau)\| \leq \kappa\tau^{-\alpha} \quad (13)$$

Theorem

The error for the splitting methods is given as :

$$\|e_1\| = K\|B\|\tau\|e_0\| + O(\tau^2) \quad (14)$$

and hence

$$\|e_2\| = K\|B\|\|e_0\|\tau^{1+\alpha} + O(\tau^{2+\alpha}), \quad (15)$$

where A is unbounded and B is bounded.

Proof :

For e_1 we have :

$$c_1(\tau) = \exp(A\tau)u_n \quad (16)$$

$$c(\tau) = \exp((A + B)\tau)u_n = \exp(A\tau) \quad (17)$$

$$+ \int_{t^n}^{t^{n+1}} \exp(As)B \exp((t^{n+1} - s)(A + B))u_n ds$$

We obtain :

$$\begin{aligned} \|e_1\| &= \|c - c_1\| \leq \| \exp((A + B)\tau)u_n - \exp(A\tau) \| \quad (18) \\ &\leq \|B\| \tau u_n \end{aligned}$$

For e_2 we have :

$$\begin{aligned}
 c_2(\tau) &= \exp(B\tau)u_n \\
 &+ \int_{t^n}^{t^{n+1}} \exp(Bs)A \exp((t^{n+1} - s)A)u_n ds \quad (19)
 \end{aligned}$$

$$\begin{aligned}
 c(\tau) &= \exp(B\tau) + \int_{t^n}^{t^{n+1}} \exp(Bs)A \exp((t^{n+1} - s)A)u_n ds \\
 &+ \int_{t^n}^{t^{n+1}} \exp(Bs)A \quad (20) \\
 &\int_{t^n}^{t^{n+1}-s} \exp(A\rho)B \exp((t^{n+1} - s - \rho)(A + B))u_n d\rho ds
 \end{aligned}$$

We obtain :

$$\begin{aligned} \|e_2\| &\leq \| \exp((A + B)\tau)u_n - c_2 \| & (21) \\ &\leq \|B\| \tau^{1+\alpha} u_n \end{aligned}$$

The same idea can be done with $A = \nabla D \nabla$ $B = -\mathbf{v} \cdot \nabla$, so that one operator is less unbounded but we reduce the convergence order

$$\|e_1\| = K \|B\| \tau^\beta \|e_0\| + O(\tau^{1+\beta}) \quad (22)$$

and hence

$$\|e_2\| = K \|B\| \|e_0\| \tau^{1+\alpha+\beta} + O(\tau^{1+\alpha+\beta}), \quad (23)$$

where $0 \leq \alpha, \beta < 1$.

Proof-idea submitted to CAM, Elsevier, April 2008.

Stability with full discretization in time and space

In the discrete case we can balance the loose of regularity. We assume the two stages for the iterative method and discretised with a θ -method:

$$\begin{aligned}\bar{c}_{i+1}^{n+1} &= c_i^n + \tau(1 - \theta_1)(A(c_{i+1}^n) + B(c_i^n)) \\ &\quad + \tau\theta_1(A(\bar{c}_{i+1}^{n+1}) + B(c_i^{n+1})),\end{aligned}\tag{24}$$

$$\begin{aligned}c_{i+1}^{n+1} &= c_{i+1}^n + \tau(1 - \theta_2)(A(c_{i+1}^n) + B(c_{i+1}^n)) \\ &\quad + \tau\theta_2(A(\bar{c}_{i+1}^{n+1}) + B(c_{i+1}^{n+1})),\end{aligned}\tag{25}$$

where $c_i^n = c_{i+1}^n = c^n$ and the initialisation with $c_0^{n+1} = c^n$

For the linear system we denote $Z_1 = \tau A$ and $Z_2 = \tau B$ and we set $\theta_1 = \theta_2$.

We get the following stability equation, cf. [Hundsdofer 2005] and for $\theta = 1/2$. For the first iteration $i = 1$ and get

$$\begin{aligned}
 c_1^{n+1} &= (I + (I - 1/2Z_2)^{-1}(I - 1/2Z_1)^{-1}(Z_1 + Z_2))c^n, & (26) \\
 &= (I - 1/2Z_2)^{-1}((I - 1/2Z_2) + (I - 1/2Z_1)^{-1}(Z_1 + Z_2))c^n \\
 &= (I - 1/2Z_2)^{-1}(I - 1/2Z_1)^{-1}(I + 1/2Z_1)(I + 1/2Z_2)c^n \\
 c_1^{n+1} &= R_1(Z_1, Z_2)c^n \\
 &= R_{impl.Euler}(1/2Z_2)R_{CN}(Z_1)R_{exp.Euler}(1/2Z_2)c^n
 \end{aligned}$$

where we have the time-restriction for the explicit Euler method.
 Can we improve the stability with implicit methods ?

To balance the method and improve the stability, we suggest a prestepping for c^n , e.g. additional implicit steps. We suggest the following algorithm.

Hence, we will get:

$$c_1^{n+1} = R_1(Z_1, Z_2)R_2(Z_2)c^{n-1/2} \quad (27)$$

$$= (I - 1/2Z_2)^{-1}(I - 1/2Z_1)^{-1}(I + 1/2Z_1)(I + 1/2Z_2) \quad (28)$$

$$(I - 1/2Z_2)^{-1}(I - 1/2Z_1)^{-1}c^{n-1/2}$$

$$= R_{impl.Euler}(1/2Z_2)R_{CN}(Z_1)R_{CN}(Z_2)R_{impl.Euler}(1/2Z_1)c^{n-1/2}$$

where $R_{impl.Euler}$ and R_{CN} are the stability function of implicit Euler and Crank-Nicolson method. So we can stabilise the scheme with a prestep $1/2\tau$ that is based on an implicit method, with the initial value $c^{n-1/2}$.

Proof is submitted to Elsevier Nov. 2007.

Transport-Reaction Models

First example : 2D Diffusion-Reaction equation

We deal with the time dependent 2-D equation:

$$\partial_t u(x, y, t) = u_{xx} + u_{yy} - 4(1 + y^2)e^{-t}e^{x+y^2} \quad (29)$$

$$u(x, y, 0) = e^{x+y^2} \text{ in } \Omega = [-1, 1] \times [-1, 1] \quad (30)$$

$$u(x, y, t) = e^{-t}e^{x+y^2} \text{ on } \partial\Omega \quad (31)$$

with exact solution

$$u(x, y, t) = e^{-t}e^{x+y^2} \quad (32)$$

We choose the time interval $[0, 1]$ and again use Finite Differences for the space with $\Delta x = 2/19$.

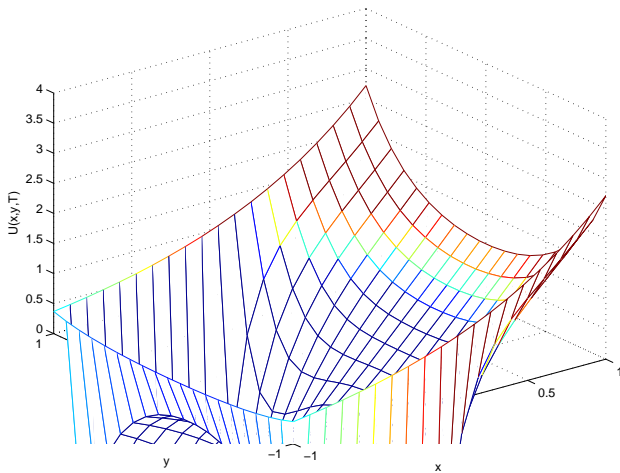
We define our operators by splitting the plane into two halves.

We choose one splitting interval.

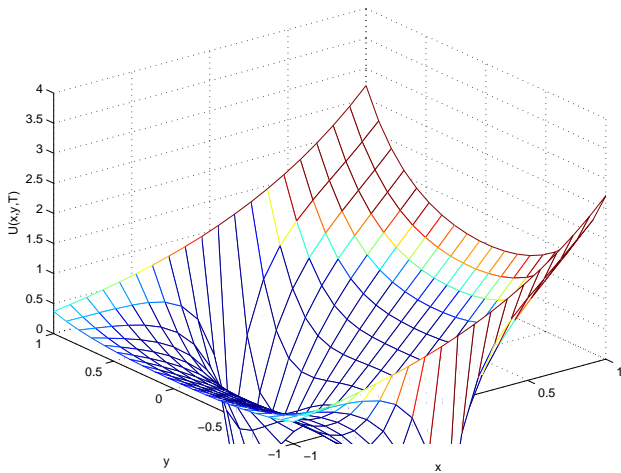
Iterative steps	Number of splitting-partitions	Max-error
1	1	2.7183e+000
2	1	8.2836e+000
3	1	3.8714e+000
4	1	2.5147e+000
5	1	1.8295e+000
10	1	6.8750e-001
15	1	2.5764e-001
20	1	8.7259e-002
25	1	2.5816e-002
30	1	5.3147e-003
35	1	2.8774e-003

Table: Numerical results for the first example with the Iterative Operator Splitting method and BDF3 with $h = 10^{-1}$.

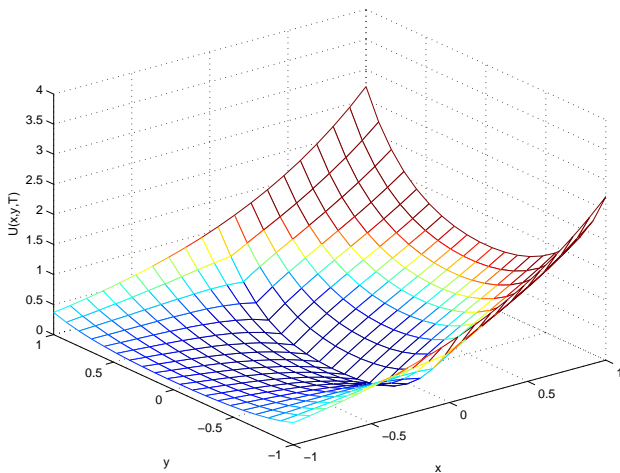
Relaxation of the model



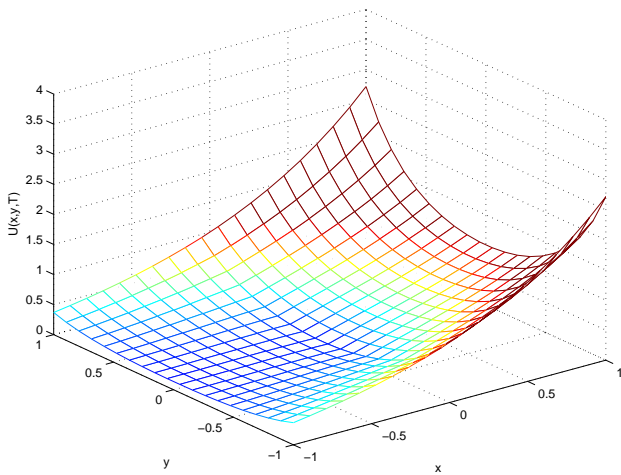
Relaxation of the model



Relaxation of the model



Relaxation of the model



Test example 2: Burgers equation

We deal with a 2D example where we can derive an analytical solution.

$$\partial_t u = -u \partial_x u - u \partial_y u + \mu(\partial_{xx} u + \partial_{yy} u) + f(x, y, t), \quad (33)$$

$$(x, y, t) \in \Omega \times [0, T]$$

$$u(x, y, 0) = u_{\text{ana}}(x, y, 0), \quad (x, y) \in \Omega \quad (34)$$

$$\text{with } u(x, y, t) = u_{\text{ana}}(x, y, t) \text{ on } \partial\Omega \times [0, T], \quad (35)$$

where $\Omega = [0, 1] \times [0, 1]$, $T = 1.25$, and μ is the viscosity.
The analytical solution is given as

$$u_{\text{ana}}(x, y, t) = \left(1 + \exp\left(\frac{x + y - t}{2\mu}\right)\right)^{-1}, \quad (36)$$

where $f(x, y, t) = 0$.

The operators are given as:

$A(u)u = -u\partial_x u - u\partial_y u$, hence $A(u) = -u\partial_x - u\partial_y$ (the nonlinear operator),

$Bu = \mu(\partial_{xx}u + \partial_{yy}u) + f(x, y, t)$ (the linear operator).

We apply the nonlinear Algorithm ?? to the first equation and obtain

$A(u_{i-1})u_i = -u_{i-1}\partial_x u_i - u_{i-1}\partial_y u_i$ and

$Bu_{i-1} = \mu(\partial_{xx} + \partial_{yy})u_{i-1} + f$,

and we obtain linear operators, because u_{i-1} is known from the previous time step.

In the second equation we obtain by using Algorithm ??:

$A(u_{i-1})u_i = -u_{i-1}\partial_x u_i - u_{i-1}\partial_y u_i$ and

$Bu_{i+1} = \mu(\partial_{xx} + \partial_{yy})u_{i+1} + f$,

and we have also linear operators.

We have the following results, see Tables 2, for different steps in time and space and different viscosities.

$\Delta x = \Delta y$	Δt	err_{L_1}	err_{\max}	ρ_{L_1}	ρ_{\max}
1/10	1/10	0.0549	0.1867		
1/20	1/10	0.0468	0.1599	0.2303	0.2234
1/40	1/10	0.0418	0.1431	0.1630	0.1608
1/10	1/20	0.0447	0.1626		
1/20	1/20	0.0331	0.1215	0.4353	0.4210
1/40	1/20	0.0262	0.0943	0.3352	0.3645
1/10	1/40	0.0405	0.1551		
1/20	1/40	0.0265	0.1040	0.6108	0.5768
1/40	1/40	0.0181	0.0695	0.5517	0.5804

Table: Numerical results for the Burgers equation with viscosity $\mu = 0.05$, initial condition $u_0(t) = c_n$, and two iterations per time step.

Figure 2 presents the profile of the 2D nonlinear Burgers equation.

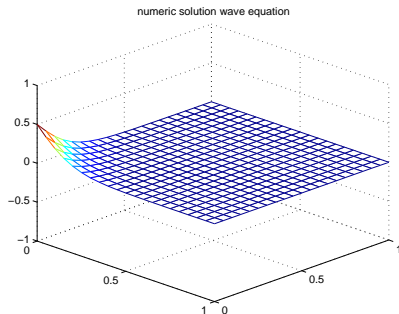


Figure: Burgers equation at initial time $t = 0.0$ for viscosity $\mu = 0.05$.

Figure 2 presents the profile of the 2D nonlinear Burgers equation.

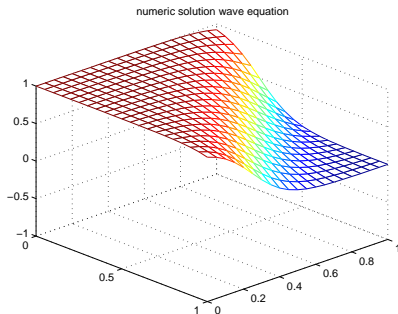


Figure: Burgers equation at end time $t = 1.25$ for viscosity $\mu = 0.05$.

FutureWorks

Outview

- 1) Global Consistency and Stability for the iterative splitting method, e.g. did we receive an tremendous reduction of order, e.g. one or two orders.
- 2) Decomposition ideas with respect to the eigenvalues of the discretized operators.
- 3) Consistency and Stability for the nonlinear splitting methods.