



Research Seminar, Department of Computer
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Lecture: Decomposition Methods

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Outline of the talk

- 0) Motivation Modelling Part : Material-Research and Wave Propagation
- 1) Mathematical Part : Decomposition methods
- 1.1) Consistency and Stability of Iterative Operator Splitting Methods
- 1.2) Nonlinear Ideas for the splitting methods
- 2) Unifying Theory for Iterative and Relaxation Schemes
- 3) Numerical Results

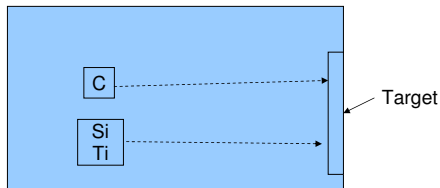
Optimisation of the deposition process: Source ideas

Based on three sources: C, Ti and Si

we like to deposit a MAX-phase material Ti_3SiC_2 .

$$0 \leq t_{Si,Ti} \leq 10^8$$

$$6.7 * 10^7 \leq t_C \leq 10^8$$



First numerical Results of the Deposition process

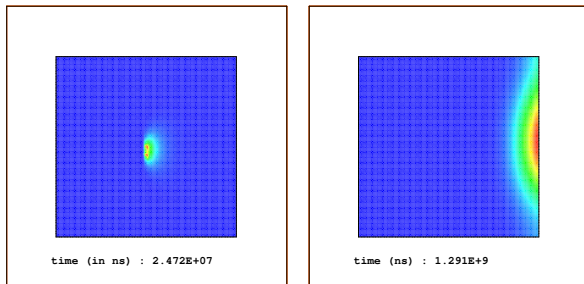


Figure: Source is moving in y direction with step 5 .

Deposition Rate

We present the deposition rates of the first experiment of the single source.

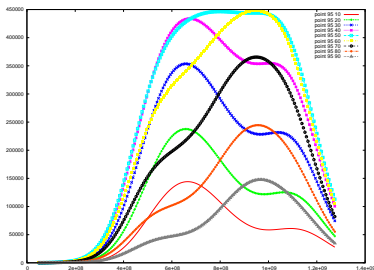


Figure: Source is moving in y direction with step 5 .

Material Model: Deposition Process

- Macro-Scale Models : Simulation of the Gas-Transport through the chamber
- Micro-Scale Models :
 - CVD-Method : Simulation of the Vaporisation (solid-vapor) process
 - PVD-Method (Sputtering): Simulation of the ion-interaction (plasma simulation)
 - PVD-Method (Sputter Deposition) : Simulation of the Topology of the surface (e.g. Level set method)

Macro-Scale Model : (Small Knudsen Numbers, Far Field Model)

For this model we can assume a continuum flow, and the fluid equations can be treated with a Navier-Stokes or especially with a reaction-diffusion equation.

$$\frac{\partial}{\partial t} \mathbf{c} + \nabla \cdot \mathbf{F} - R_g = 0, \text{ in } \Omega \times [0, T] \quad (1)$$

$$\mathbf{F} = \mathbf{v}\mathbf{c} - D\nabla\mathbf{c},$$

$$\mathbf{c}(x, t) = \mathbf{c}_0(x), \text{ on } \Omega, \quad (2)$$

$$\mathbf{c}(x, t) = \mathbf{c}_1(x, t), \text{ on } \partial\Omega \times [0, T], \quad (3)$$

where c is the molar concentration and F the flux of the species. v is the velocity, D is the diffusivity matrix and R_g is the reaction term. $Kn = \frac{\lambda}{L}$ (free path of molecules).

Micro-Scale Model : Simulation of the Vaporisation (CVD-method)

The vaporisation can be modeled with a heat conduction equation :

$$\rho(T)C(T)\partial_t T - \nabla k(T)\nabla T = Q(x, t), \text{ in } \Omega \times [0, T] \quad (4)$$

$$T(x, t) = T_0(x), \text{ on } \Omega, \quad (5)$$

$$T(x, t) = T_1(x, t), \text{ on } \partial\Omega \times [0, T], \quad (6)$$

where T is the temperatur distribution, ρ the mass density, k the thermal conductivity, C the specitif heat. The source term Q represents the laser energy.

The flow of material can be modeled by the Hertz-Knudsen equation and we can derive the ablation rate :

$$v(T) = (1 - \beta) \sqrt{m / (2\pi k_b T)} p / p_0 \exp(l_v / k_b (\frac{1}{T_B} - \frac{1}{T})), \quad (7)$$

where T_B is the boiling temperature, k_b the Boltzmann constant, β the back flux coefficient and l_v the latent heat of the vaporisation of the material.

Micro-Scale Model : Ion Interaction (Large Knudsen Numbers, Near Field Model)

The model assumes that the heavy particles can be described with a dynamical fluid model, where the elastic collisions define the dynamics and few inelastic collisions are, among other reasons, responsible for the chemical reactions.

Model for Large Knudsen Numbers (Near Field Model)

The Boltzmann equation for heavy particles (ions and neutral elements) is now given as

$$\frac{\partial}{\partial t} n_s + \frac{\partial}{\partial \mathbf{r}} \cdot (n_s \mathbf{u} + n_s \mathbf{c}_s) = Q_n^{(s)}, \quad (8)$$

$$\frac{\partial}{\partial t} \rho \mathbf{u} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{u} \mathbf{u} + n T \underline{\underline{I}} - \underline{\underline{\tau}}^*) = \sum_{s=1}^N q_s n_s \langle \mathbf{E} \rangle, \quad (9)$$

$$\frac{\partial}{\partial t} \mathcal{E}_{\text{tot}}^* + \frac{\partial}{\partial \mathbf{r}} \cdot (\mathcal{E}_{\text{tot}}^* \mathbf{u} + \mathbf{q}^* + n T \mathbf{u} - \underline{\underline{\tau}}^* \cdot \mathbf{u}) = \sum_{s=1}^N q_s n_s (\mathbf{u} + \mathbf{c}_s) \cdot \langle \mathbf{E} \rangle - Q_{\mathcal{E}, \text{inel}}^{(e)}, \quad (10)$$

Model for Large Knudsen Numbers (Near Field Model)

where ρ denotes the mass density, \mathbf{u} is the velocity, and T the temperature of the ions. $\mathcal{E}_{\text{tot}}^*$ is the total energy of the heavy particles.

Application to Model-Problem : Wave Action Equation

Idea : Modelling of Wave-propagation (wave-travelling plus wind-terms)

$$\begin{aligned} \partial_t N + \partial_x(c_x N) + \partial_y(c_y N) \\ + \partial_\sigma(c_\sigma N) + \partial_\theta(c_\theta N) = S_{tot}, \text{ in } \Omega \times [0, T], \end{aligned} \quad (11)$$

$$N = N_{Dirich}, \text{ on } \partial\Omega_{Dirich} \times [0, T], \quad (12)$$

$$\mathbf{v} \cdot \mathbf{n} N = h_{flux}, \text{ on } \partial\Omega_{flux} \times [0, T] \quad (13)$$

where $N = N(t, x, y, \sigma, \theta)$ is the wave density spectrum, t time, c_x and c_y are the wave propagation velocities in x and y space, c_σ and c_θ are the wave propagation velocities in σ and θ , σ is the relative frequency and θ is the wave direction.

$\mathbf{v} = (c_x, c_y, c_\sigma, c_\theta)^t$ is the velocity, h_{flux} is the flux function. S_{tot} is the total source term.

Idea : Treatment of the different physical behaviour.

- Transport-Scale : Discretisation with Characteristic Method, (Eulerian Schemes)
- Source-Scale Models :
 - Nonlinear Term: Explicit and iterative methods for the linearisation
 - Linear Term: Implicit discretization methods (Lagrangian Schemes)

Decoupling with respect to the different schemes.

Decomposition: Introduction

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

- 1 Transport-Reaction Processes, see [Geiser2006] [Hundsdoerfer, Verwer 2003](Physical splitting);
- 2 Hamiltonian Systems, see [McLachlan94], [Hairer, Lubich, Wanner 02] (Symplectic splitting).
- 3 Air pollutant models, see [Zlatev95] (Operator Splitting)
- 4 Wave propagation models, see [Roger et al 1999] (Wave action model)
- 5 Maxwell equations, see [Horvath06] (Operator Splitting)

Introduction

Methods of decomposition

- Time- and Spatial-decomposition methods:

Contribution with the decomposition

- Decoupling the time-scales, space-scales. (Reduce the stiffness in single operators).
- Decoupling the multi-physics. (Reduce the unphysical behaviour with best choice of discretization and solver methods)
- Time-adaptivity, Space-adaptivity. (Efficiency and accuracy in computational)
- Parallelization in Time and Space. (Reduction of computational time)

Results : More efficient and fast algorithms with high accuracy, simple implementable.

Classical Splitting Methods

Fractional Step (or A-B splitting of first order splitting)

$$\frac{N^{n+1/4} - N}{\Delta t} + \partial_x(c_x N) + \partial_y(c_y N) = 0, \quad (14)$$

$$\frac{N^{n+2/4} - N^{n+1/4}}{\Delta t} + \partial_\theta(c_\theta N) = 0, \quad (15)$$

$$\frac{N^{n+3/4} - N^{n+2/4}}{\Delta t} + \partial_\sigma(c_\sigma N) = 0, \quad (16)$$

$$\frac{N^{n+1} - N^{n+3/4}}{\Delta t} = S_{tot}, \quad (17)$$

where we have included the boundary conditions, $N = N^n$ and we can apply separate methods for each step.

Problems of the Classical Splitting Methods

1.) Error analysis

Error is of first order global in time :

Local and global error for the decomposition and the full solution

$$e(N) = N_{num}(t^{n+1}) - N_{exact}(t^{n+1}) , \text{ local error}$$

$$e(N)/\tau = \frac{1}{2}\tau((BA - AB) + (CA - AC) + (DA - AD) \\ + (CB - BC) + (DB - BD) + (DC - CD))c(t^n) + O(\tau^2) ,$$

$O(\tau)$ as global error, for $A = -\partial_x c_x - \partial_y c_y$, $B = -\partial_\theta c_\theta$,
 $C = -\partial_\sigma c_\sigma$, $D = S_{tot}$ not commuting, otherwise one get exact results, where $\tau = t^{n+1} - t^n$, [Strang 68].

2.) Physical Error :

In each equation, we solve a different problem due to the full equation, e.g. no influence of the intermediate time-steps to the other equations.

$$\partial_t N_1 = A N_1, \text{ with } N_1^n = N^n \quad (18)$$

$$\partial_t N_2 = B N_2, \text{ with } N_2^n = N_1^{n+1}, \quad (19)$$

We only interact at the initial conditions, so time-scale of operator A and B are independent and therefore not an interaction, e.g. coupled transport equations [Geiser 07].

Iterative Operator Splitting Methods

Benefits of iterative splitting methods

- Larger time-steps are possible in each iterative step
- Spectrum of the operator allow to control the stiffness of the operators
- Higher order can be claimed with more iterative steps
- Efficient and simple implementation of the iterative schemes
- Parallel algorithms can be used

Application to the Wave Action Equation

We solve iteratively four equations:

$$\begin{aligned}\partial_t N_i &= -\partial_x(c_x N_i) - \partial_y(c_y N_i) - \partial_\theta(c_\theta N_{i-1}) - \partial_\sigma(c_\sigma N_{i-1}) + S_{i-1,tot}, \\ \partial_t N_{i+1} &= -\partial_x(c_x N_i) - \partial_y(c_y N_i) - \partial_\theta(c_\theta N_{i+1}) - \partial_\sigma(c_\sigma N_{i-1}) + S_{i-1,tot}, \\ \partial_t N_{i+2} &= -\partial_x(c_x N_i) - \partial_y(c_y N_i) - \partial_\theta(c_\theta N_{i+1}) - \partial_\sigma(c_\sigma N_{i+2}) + S_{i-1,tot}, \\ \partial_t N_{i+3} &= -\partial_x(c_x N_i) - \partial_y(c_y N_i) - \partial_\theta(c_\theta N_{i+1}) - \partial_\sigma(c_\sigma N_{i+2}) + S_{i+3,tot},\end{aligned}$$

where $i = 1, 2, 3, \dots$, $N_0 \equiv 0$, and $N_i^n = N^n$, the stop-criterion is given as $\|N_i^{n+1} - N_{i-1}^{n+1}\| \leq \text{err}$.

Analysis: Iterative Operator Splitting Methods

We concentrate on two operators:

$$\frac{\partial c_i(t)}{\partial t} = A c_i(t) + B c_{i-1}(t), \text{ with } c_i(t^n) = u^n, \quad (20)$$

$$\frac{\partial c_{i+1}(t)}{\partial t} = A c_i(t) + B c_{i+1}(t), \text{ with } c_{i+1}(t^n) = u^n, \quad (21)$$

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 $c_{\text{sp}}^{n+1} = c_{2m+1}(t^{n+1})$. (Clearly, the functions $c_k(t)$ ($k = i - 1, i, i + 1$) depend on the interval $[t^n, t^{n+1}]$, too, but, for the sake of simplicity, in our notation we omit the dependence on n .)

Numerical Analysis of the iterative Scheme :

- Consistency (local error)
- Stability (Boundedness of the operators)

Iterative Splitting Schemes

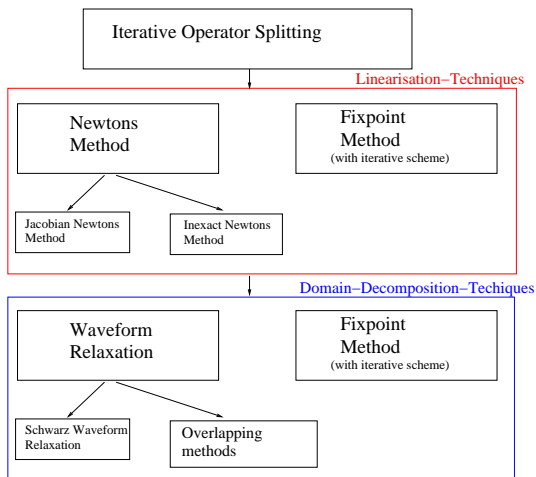


Figure: Iterative Splitting Methods

Error for the Iterative splitting-method

Theorem

The error for the splitting methods is given as :

$$\|e_i\| = K\|B\|\tau_n\|e_{i-1}\| + O(\tau_n^2) \quad (22)$$

and hence

$$\|e_{2m+1}\| = K_m\|e_0\|\tau_n^{2m} + O(\tau_n^{2m+1}), \quad (23)$$

where τ_n 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 . First we assume A and B are bounded, monotone operators. The error can be controlled by the operator B , e.g. non stiff operator.

Proof : Taylor-expansion and estimation of exp-functions. See the work Geiser, Farago (2005).

Error of the iterative method for bounded operators

Theorem

The error for the splitting methods is given as :

$$\|e_i\| = K\|B\|\tau\|e_{i-1}\| + O(\tau^2) \quad (24)$$

and hence

$$\|e_{2m+1}\| = K_m\|e_0\|\tau^{2m} + O(\tau^{2m+1}), \quad (25)$$

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, e.g. spatial discretised operators, we loose smoothness in the differential formulation, see :

$$\frac{\partial c_1}{\partial t} = Ac_1 + Bc_0, c_1 \in C^k(H^s(\Omega) \times [0, T]), \quad (26)$$

$$\frac{\partial c_2}{\partial t} = Ac_1 + Bc_2, c_2 \in C^k(H^{s-2}(\Omega) \times [0, T]), \quad (27)$$

$$\frac{\partial c_3}{\partial t} = Ac_3 + Bc_2, c_3 \in C^k(H^{s-1}(\Omega) \times [0, T]), \quad (28)$$

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

Solution : Integral formulation with variation of constants can bound our operators and time-space discretization to obtain a stable method.

Error of the iterative method for unbounded operators

Integral-Formulation and application of the variation of constant formula:

$$\begin{aligned} \exp((A + B)\tau)c_n &= \exp(A\tau) \\ &+ \int_{t^n}^{t^{n+1}} \exp(As)B \exp((t^{n+1} - s)(A + B))u_n ds \end{aligned} \quad (29)$$

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

$$\|A^\alpha \exp(A\tau)\| \leq \kappa\tau^{-\alpha} \quad (30)$$

$$\|A^\alpha \exp((A + B)\tau)\| \leq \kappa\tau^{-\alpha} \quad (31)$$

where exp-operators are bounded.

Theorem

The error for the splitting methods is given as :

$$\|e_1\| = K\|B\|\tau\|e_0\| + O(\tau^2) \quad (32)$$

and hence

$$\|e_2\| = K\|B\|\|e_0\|\tau^{1+\alpha} + O(\tau^{2+\alpha}), \quad (33)$$

where A is unbounded and B is bounded.

Proof :

For e_1 we have :

$$c_1(\tau) = \exp(A\tau)u_n \quad (34)$$

$$c(\tau) = \exp((A + B)\tau)u_n = \exp(A\tau) \quad (35)$$

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

We obtain :

$$\|e_1\| = \|c - c_1\| \leq \|\exp((A + B)\tau)u_n - \exp(A\tau)\| \quad (36)$$

$$\leq \|B\|\tau u_n \quad (37)$$

For e_2 we have :

$$c_2(\tau) = \exp(B\tau)u_n + \int_{t^n}^{t^{n+1}} \exp(Bs)A \exp((t^{n+1} - s)A)u_n ds \quad (38)$$

$$c(\tau) = \exp(B\tau) + \int_{t^n}^{t^{n+1}} \exp(Bs)A \exp((t^{n+1} - s)A)u_n ds + \int_{t^n}^{t^{n+1}} \exp(Bs)A \int_{t^n}^{t^{n+1}-s} \exp(A\rho)B \exp((t^{n+1} - s - \rho)(A + B))u_n d\rho ds \quad (39)$$

We obtain :

$$\|e_2\| \leq \|\exp((A + B)\tau)u_n - c_2\| \quad (40)$$

$$\leq \|B\|\tau^{1+\alpha}u_n \quad (41)$$

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

$$\|e_1\| = K\|B\|\tau^\beta\|e_0\| + O(\tau^{1+\beta}) \quad (42)$$

and hence

$$\|e_2\| = K\|B\|\|e_0\|\tau^{1+\alpha+\beta} + O(\tau^{1+\alpha+\beta}), \quad (43)$$

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

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

Stability and Conservation of the differentiability

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:

$$\begin{aligned}\bar{c}_{i+1}^{n+1} &= c_i^n + \tau(1 - \theta_1)(A(c_{i+1}^n) + B(c_i^n)) \\ &\quad + \tau\theta_1(A(\bar{c}_{i+1}^{n+1}) + B(c_i^{n+1})),\end{aligned}\tag{44}$$

$$\begin{aligned}c_{i+1}^{n+1} &= c_{i+1}^n + \tau(1 - \theta_2)(A(c_{i+1}^n) + B(c_{i+1}^n)) \\ &\quad + \tau\theta_2(A(\bar{c}_{i+1}^{n+1}) + B(c_{i+1}^{n+1})),\end{aligned}\tag{45}$$

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 $\theta = 1/2$: We compute the first iteration with $i = 1$ and get the equation

$$\begin{aligned}c_1^{n+1} &= (I + (I - 1/2Z_2)^{-1}(I - 1/2Z_1)^{-1}(Z_1 + Z_2))c^n, & (46) \\ &= (I - 1/2Z_2)^{-1}((I - 1/2Z_2) + (I - 1/2Z_1)^{-1}(Z_1 + Z_2))c^n \\ &= (I - 1/2Z_2)^{-1}(I - 1/2Z_1)^{-1}(I + 1/2Z_1)(I + 1/2Z_2)c^n \\ c_1^{n+1} &= R_1(Z_1, Z_2)c^n\end{aligned}$$

To improve this method we suggest to do a prestepping for c_0^n , which means that we define c_0^n from the known value c^n with a suitably chosen stable method. Namely, we suggest the following algorithm.

Hence, we will get:

$$c_1^{n+1} = R_1(Z_1, Z_2)R_2(Z_2)c^{n-1/2} \quad (47)$$

$$= (I - 1/2Z_2)^{-1}(I - 1/2Z_1)^{-1}(I + 1/2Z_1)(I + 1/2Z_2) \quad (48)$$

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

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

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.

Ideas for Nonlinear Splitting Methods

The iterative operator-splitting method is used as a fixed-point scheme or with embedded Newton's method to linearize the nonlinear operators.

We concentrate again on nonlinear differential equations of the form

$$\frac{du}{dt} = A(u(t))u(t) + B(u(t))u(t), \quad \text{with } u(t^n) = u^n, \quad (49)$$

where $A(u), B(u)$ are matrices with nonlinear entries and densely defined, where we assume that the entries involve the spatial derivatives of c .

Iterative operator-splitting method as fixed-point scheme

We split our nonlinear differential equation (49) by applying

$$\frac{du_i(t)}{dt} = A(u_{i-1}(t))u_i(t) + B(u_{i-1}(t))u_{i-1}(t), \quad (50)$$

$$\text{with } u_i(t^n) = c^n,$$

$$\frac{du_{i+1}(t)}{dt} = A(u_{i-1}(t))u_i(t) + B(u_{i-1}(t))u_{i+1}(t), \quad (51)$$

$$\text{with } u_{i+1}(t^n) = c^n,$$

where the time step is $\tau = t^{n+1} - t^n$. The iterations are $i = 1, 3, \dots, 2m + 1$. $u_0(t) = c_n$ is the starting solution, where we assume that the solution c^{n+1} is near c^n , or $u_0(t) = 0$. So we have to solve the local fixed-point problem. c^n is the known split approximation at time level $t = t^n$.

Consistency and Stability Proofs :

1.) Bounded case : First linearisation, then application of the linear theory.

2.) Unbounded Case : Linearisation and Discretisation in time and space, then application of the discrete theory.

Unifying Theory : Waveform-Relaxation and Iterative Splitting Method

- Reduction to a unified method (Iterative and Relaxation).
- Application of the convergence proof for the unified method.

Waveform-Relaxation Method:

$$\frac{du_j}{dt} = Pu_j + Qu_{j-1} + f, \quad (52)$$

$$u_j(t^n) = u(t^n), \quad (53)$$

where $A = P + Q$, e.g. P is the diagonal part of A (Jacobi-method).

Here the splitting method is done abstract with respect to the matrix A . The method considered an effective solver method with respect to the underlying matrices.

Iterative Operator Splitting Method:

$$\frac{du_j}{dt} = Pu_j + Qu_{j-1} + f, \quad (54)$$

$$u_j(t^n) = u(t^n), \quad (55)$$

$$\frac{du_{j+1}}{dt} = Pu_j + Qu_{j+1} + f, \quad (56)$$

$$u_{j+1}(t^n) = u(t^n), \quad (57)$$

where P, Q are matrices given by spatial discretisation, e.g. P is the convection part of Q the diffusion part.

But we can also do an abstract decomposition, take into account $A = P + Q$, where P is the matrix with small eigenvalues and Q is the matrix with large eigenvalues.

Unifying Theory:

As iterative splitting method we have at least 2 waveform itative methods :

- 1.) Inner Iteration
- 2.) Outer Iteration

Unified Relaxation Method:

Outer Iteration :

$$\frac{dU_i}{dt} = \mathcal{P}U_i + \mathcal{Q}U_{i-1} + F, \quad (58)$$

$$U_i(t^n) = U(t^n), \quad (59)$$

where \mathcal{P} and \mathcal{Q} are the diagonal and outerdiagonal matrices of the splitting methods.

Inner Iteration:

$$\frac{du_j}{dt} = Pu_j + Qu_{j-1} + f, \quad (60)$$

$$u_j(t^n) = u(t^n), j = 1, \dots, J \quad (61)$$

$$\frac{du_k}{dt} = Pu_J + Qu_k + f, \quad (62)$$

$$u_k(t^n) = u(t^n), k = 1, \dots, K \quad (63)$$

Unifying Analysis:

Application of an alternative waveform-relaxation scheme.

- 1.) Convergence of the inner iterations
- 2.) Convergence of the outer iterations

Transport-Reaction Models

First example : 2D Diffusion-Reaction equation

We deal with the time dependent 2-D equation:

$$\partial_t u(x, y, t) = u_{xx} + u_{yy} - 4(1 + y^2)e^{-t}e^{x+y^2} \quad (64)$$

$$u(x, y, 0) = e^{x+y^2} \text{ in } \Omega = [-1, 1] \times [-1, 1] \quad (65)$$

$$u(x, y, t) = e^{-t}e^{x+y^2} \text{ on } \partial\Omega \quad (66)$$

with exact solution

$$u(x, y, t) = e^{-t}e^{x+y^2} \quad (67)$$

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

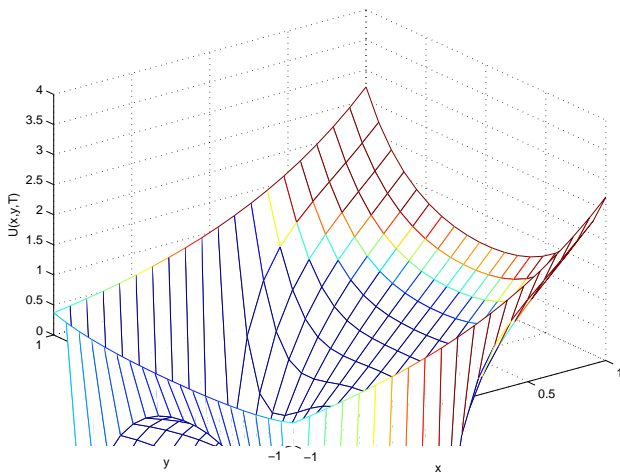
We define our operators by splitting the plane into two halves.

We choose one splitting interval.

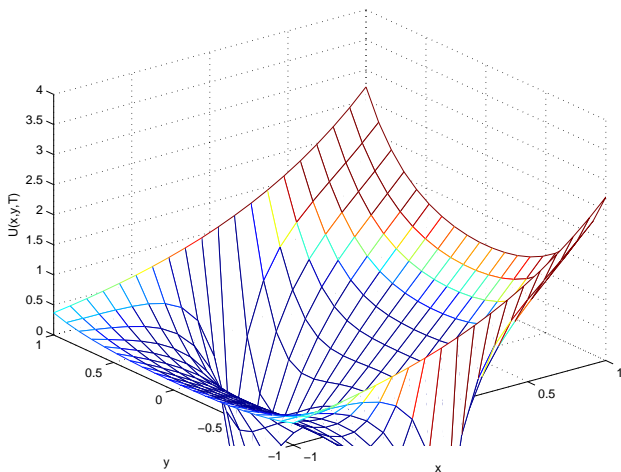
Iterative steps	Number of splitting-partitions	Max-error
1	1	2.7183e+000
2	1	8.2836e+000
3	1	3.8714e+000
4	1	2.5147e+000
5	1	1.8295e+000
10	1	6.8750e-001
15	1	2.5764e-001
20	1	8.7259e-002
25	1	2.5816e-002
30	1	5.3147e-003
35	1	2.8774e-003

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

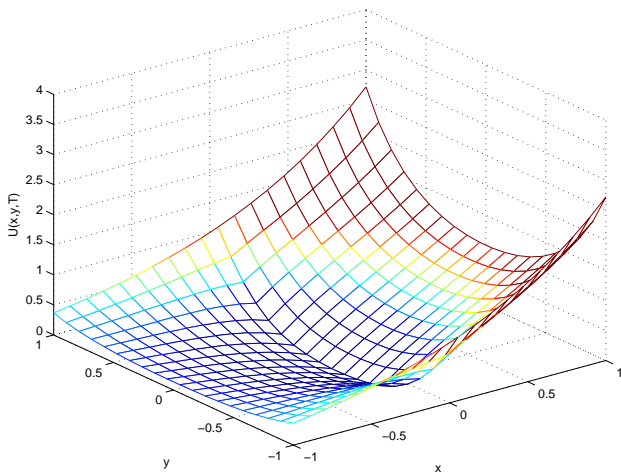
Relaxation of the model



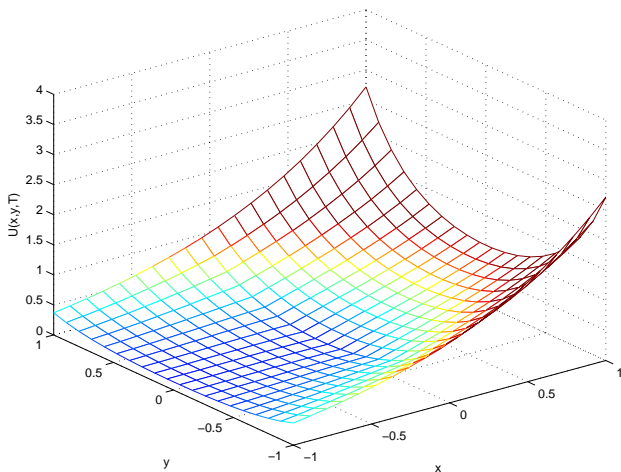
Relaxation of the model



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.

$$\partial_t u = -u \partial_x u - u \partial_y u + \mu(\partial_{xx} u + \partial_{yy} u) + f(x, y, t), \quad (68)$$

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

$$u(x, y, 0) = u_{\text{ana}}(x, y, 0), \quad (x, y) \in \Omega \quad (69)$$

$$\text{with } u(x, y, t) = u_{\text{ana}}(x, y, t) \text{ on } \partial\Omega \times [0, T], \quad (70)$$

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

$$u_{\text{ana}}(x, y, t) = \left(1 + \exp\left(\frac{x + y - t}{2\mu}\right)\right)^{-1}, \quad (71)$$

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 50 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 51:

$A(u_{i-1})u_i = -u_{i-1}\partial_x u_i - u_{i-1}\partial_y u_i$ 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 6 presents the profile of the 2D nonlinear Burgers equation.

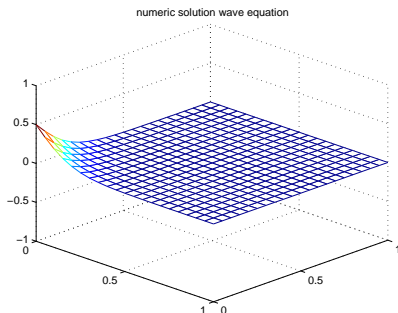


Figure: Burgers equation at initial time $t = 0.0$ for viscosity $\mu = 0.05$.

Figure 6 presents the profile of the 2D nonlinear Burgers equation.

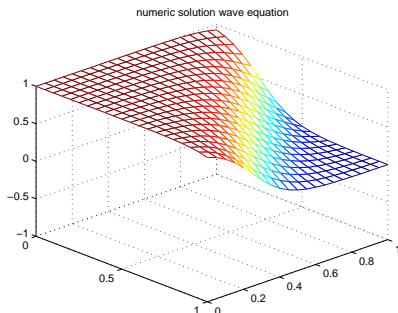


Figure: Burgers equation at end time $t = 1.25$ for viscosity $\mu = 0.05$.

Transport-Reaction Models

Second example : CVD-Modell (2D Convection-Diffusion-Reaction equation)

We deal with a gas-transport model

For this model we can assume a continuum flow, and the fluid equations can be treated with a Navier-Stokes or especially with a reaction-diffusion equation.

$$\frac{\partial}{\partial t} \mathbf{c} + \nabla \cdot \mathbf{F} - R_g = 0, \text{ in } \Omega \times [0, T] \quad (72)$$

$$\mathbf{F} = \mathbf{v} \mathbf{c} - D \nabla \mathbf{c},$$

$$c(x, t) = c_0(x), \text{ on } \Omega, \quad (73)$$

$$c(x, t) = c_1(x, t), \text{ on } \partial\Omega \times [0, T], \quad (74)$$

where c is the molar concentration and F the flux of the species. v is the velocity, D is the diffusivity matrix and R_g is the reaction term.

Transport-Reaction Models

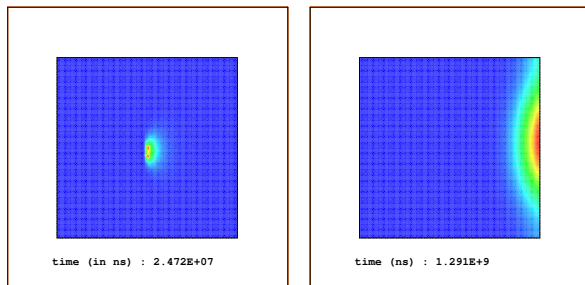


Figure: Source is moving in y direction with step 5 .

Transport-Reaction Models

In Figure 7 we present the deposition rates with a single source.

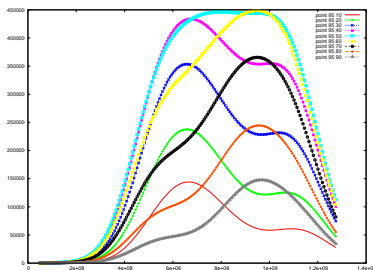
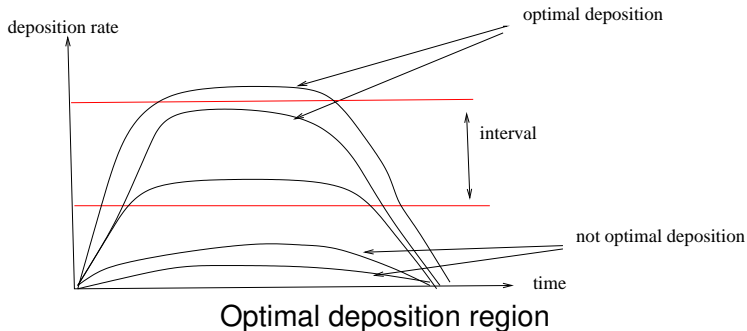


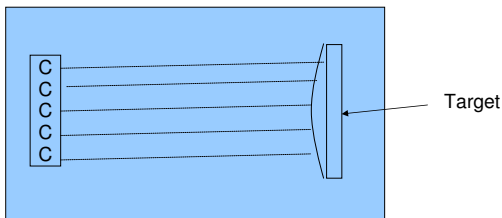
Figure: Source is moving in y direction with step 5 .

Optimisation in the deposition region

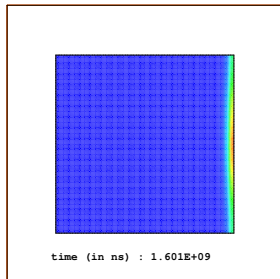
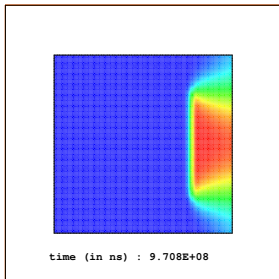
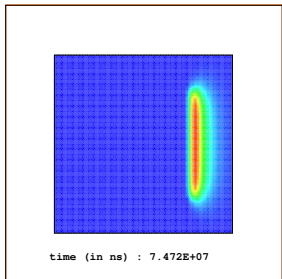


Improved Sources: Line Source

- we make two experiments, with timesteps equal to 200,250
- 1st Exp. x is between 50,55 and y is between 30,70
- 2nd Exp. x is between 75,80 and y is between 20,80

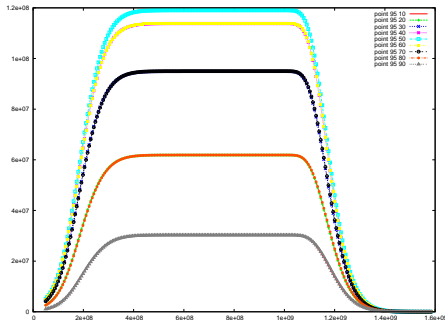


Improved Source: Line source



Line source, x is between 75,80 and y is between 20,80
with timesteps = 250

Improved Source: Line source



Deposition rates with x is between 75,80 and y is between 20,80 with timesteps = 250

FutureWorks

Outview

- 1) Simulation of a CVD process with respect to the kinetics of the reactive gas.
- 2) Optimal Control of the Deposition layer.
- 3) Decomposition the deposition process, e.g. kinetic and flux processes