Jürgen Geiser

Iterative Operator-Splitting- and Waveform-Relaxation-Methods as effective Black-Box Solvers for Multi-Physical- and Multi-Scaling Problems.

ACDL-Seminar, Aerospace Computational Design Laboratory, Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA 02139, USA, 16.12.2005
1 Outline of the talk

Motivation solving complicate problems with multi-physical and multi-scale properties:

1.) Model-Equations and Examples

2.) Black-Box Methods

3.) Theory of Black-Box-Solver : Operator-Splitting-, Waveform-Relaxation-, Domain Decomposition Method

4.) Proposed Discretisation and Solver methods

5.) Effectivity, Parallelization and Implementation

6.) Project : Waste-Disposal

7.) Project : Crystal-Growth
2 Motivation engineering-applications in Fluid-mechanics: $R^3T$
3 An engineering-application in Gas-mechanics: *WiASHiTNISE*

Stationary Temperature Field

- height = 25 cm
- \( T_{\text{min}} = 537.517 \) K
- \( T_{\text{max}} = 3312.53 \) K
- \( \Delta T_{\text{max}} = 0 \) K

heating power in crucible = 7811.89 W
heating power in coil = 2188.11 W

prescribed power = 10000 W
frequency = 10000 Hz

coil:
- 5 rings
- top = 0.18 m
- bottom = 0.02 m
4 Motivation and Ideas

Motivation:

- Complicate models in environmental science and meteorology
- Reuse of given program-code for one specific physical problem (coupling the equations, solved be different codes)
- Effectivity by solving simpler equations
- Parallelization

Ideas:

- Decoupling the equation-operators (Operator-Splitting-Methods)
- Decoupling the complicate domain (Domain-Decomposition-Methods)
- Decoupling the physical weak dependent effects
5 Model-Equation

Systems of parabolic-differential equations with first order time-derivation and second order spatial-discretisation:

\[
\frac{\partial c}{\partial t} = f(c, Ac, Bc) \text{ in } \Omega , \\
c(x, t) = g(x, t) \text{ on } \partial \Omega \text{ Boundary-Conditions} , \\
c(x, 0) = c_0(x) \text{ Initial-Condition} .
\]

where \( c = (c_1, \ldots, c_n)^t \) and \( f = (f_1, \ldots, f_n)^t \),

\[
A = \begin{pmatrix}
v_{11} \cdot \nabla c_1 & \cdots & v_{n1} \cdot \nabla c_n \\
\vdots & \ddots & \vdots \\
v_{1n} \cdot \nabla c_1 & \cdots & v_{nn} \cdot \nabla c_n
\end{pmatrix}, \quad B = \begin{pmatrix}
\nabla D_{11} \cdot \nabla c_1 & \cdots & \nabla D_{n1} \cdot \nabla c_n \\
\vdots & \ddots & \vdots \\
\nabla D_{1n} \cdot \nabla c_1 & \cdots & \nabla D_{nn} \cdot \nabla c_n
\end{pmatrix}
\]

Convection- and diffusion-operator.
6 Example: System of PDE’s in Crystal Growth: Temperature-Field and Gas-Transport

\[ \partial_t \rho_g + v_g \partial_z \rho_g + \rho_g \partial_z v_g = 0, \]  
\[ \rho_g \partial_t v_g + v_g \rho_g \partial_z v_g + R_g \partial_z \rho_g T_g = \rho_g b_g, \]  
\[ \rho_g \partial_t z_g R_g T_g + R_g \rho_g \partial_z (v_g T_g) - \nabla \cdot (\kappa_g \nabla T_g) = 0, \]  
\[ \rho_{s_i} \partial_t c_{s_i} (T_{s_i}) T_{s_i} - \nabla \cdot (\kappa_{s_i} \nabla T_{s_i}) = f_i, \]

\( \rho_g \): density, \( \kappa_g \): thermal conductivity, \( z_g \): configuration number, \( R_g \): gas constant, \( b_g \): gravity, \( \rho_{s_i} \): density, \( \kappa_{s_i} \): thermal conductivity, \( c_{s_i} \): specific heat, \( f_i \): Heat-source, \( i \)-th Solid and the boundary conditions, i.e. Two solids: normal heat flux is continuous at the interface, Gas and Solid: normal heat flux is added with the radiosity and irрадiosity, discontinuous.
7 Black-Box-Solver for the PDE-Systems

Model–Equations, Evolution–equations
(Material–Sciences
Environmental–sciences)

Transformation to a system of 2nd–order parabolic or hyperbolic equations

Decoupling and Splitting–methods

Higher order spatial discretisation–methods
Implicite higher order time–
discretisation–methods, iterative solvers

Operator–Splitting
methods (e.g. Strang–Splitting,
Iterative Operator–Splitting,
Wave–form–relaxation)

Domain–Decomposition
methods (e.g. overlapping
Schwarz wave–form relaxation)

Simpler partial–differential
equations

Simpler domains or domains of same physical parameters

Improved Discretisation and Solver methods for each equation– or domain–part,
use of developed higher order methods,
e.g. Characteristic Methods for a convection equation

Output

Solutions of complicate partial differential equations

Input: Physical relevant parameter, dominance of an equation part
Interface–Information, Scale Information

Solutions are uniqueness and exist

Splitting criteria

Not decoupable problem

e.g. strong coupled

Different scales for the equation operators

Different scales and physical behaviour in the domains

Splitting and Decoupling Theory

Developing methods for complicate equation–operators

ACDL-Seminar, Aerospace Computational Design Laboratory, Massachusetts Institute of Technology,
77 Massachusetts Ave, Cambridge, MA 02139, USA, 16.12.2005
14th December 2005 8/46
8 Multi-physical, multi-dimensional, multi-operator, multi-scale Problems

Discretisation and solver-methods for this problems are based on design of simplification of the complexity. So local discretisation-methods for all the different problem, e.g. adaptive and higher order methods or splitting-methods for decoupling into simpler problems and solve them effective and simpler.
Ideas for Coupling–Decoupling Multi–Structures (Multi–components, Multi–dimensions, Multi–physics, Multi–operators, Multi–scales)

Complicate Model with multi–structures (e.g. crystal–growth model)

Decoupled (Question: Decomposable)

Decoupling in simpler structures
Solve each simpler structure independent (extrinsic point of view)

Coupled as a multi–structure general–methods to solve all the structures (intrinsic point of view)

\[ u_1, u_2, u_3, \ldots, u_n \to u \]
Multi-Physical Methods

a.) General
Conservation Laws: Finite Volume methods (Discontinuity),
Elasticity, mechanical Properties : Finite Element methods (Continuity),
Or mixed methods.

b.) Physical Discretisation :
Flow Directions : upwinding, characteristic Methods,
Splitting of physical properties : Special Discretisation methods for each physical operator, e.g. Convection-Term is done with Characteristic-Methods. Idea of decoupling each physical operator and solve operator with adapted methods.
Physical Decoupling:

Example:

\[ \partial_t c + v \partial_x c - D \partial_{xx} c = -\lambda c \]

Discretisation (Finite Differences):

\[ \partial_t c_i = -v \frac{c_i - c_{i-1}}{\Delta x} - D \frac{c_{i+1} - c_i - 2c_i}{\Delta^2} - \lambda c_i \]

\( i \)-th node of the discretised grid.

ODE for the node \( i \):

\[ \partial_t c_i = Ac_i + Bc_i + Cc_i + f(c_{i-1}, c_{i+1}) \]

Physical relevant Parameters for the different scales:

\( A = -\frac{v}{\Delta x}, \quad B = -\frac{D}{\Delta x^2}, \quad C = -\lambda \)

e.g. strong coupling: \( A = B = C \)

weak coupling: \( A \leq C \) or \( B \leq C \), decouple in pairs: \( A + B \) and \( C \).
Multi-Scaling Methods

a.) General Solver-methods for all different scales, e.g. upscaling for an averaged scale and then a direct solver.

b.) Solver-methods for each different scale, e.g. solving on each different scale, decompose the problem into smaller scales.

Multi-Scaling–Problems

Problem exists on each scale

Decomposing in simpler scales
Higher Order for finer scales:

Multiscales in the time–distribution

Macro–scale $\rightarrow$ lower order discretisation

Micro–scale $\rightarrow$ higher order discretisation
Decomposition Methods

a.) General Solver-methods for all different domain (unique domain).

b.) Solver-methods for each different domain, e.g. solving on each different domain (adaptivity, more effectivity).

Domain Decomposition

Unique Domains

Overlapping domains

\[ \Omega \]

\[ \Omega_1 \quad \Omega_2 \quad \Omega_3 \quad \Omega_4 \quad \Omega_5 \quad \Omega_6 \]
9 **Operator-Splitting methods and Waveform-Relaxation**

History and Literature:

- ADI-methods (Alternating direction implicit), see: Peaceman-Rachford (1955)
- Strang-Marchuk-Splitting methods, see: Strang (1968)
- Iterative Operator-Splitting Methods, see: Kanney, Miller, Kelly (2003), Farago, Geiser (2005)
- Waveform-relaxation Methods, see: Vandewalle (1993)
Operator-Splitting-Method

Idea: Decoupling of complex equations in simpler equations, solving simpler equations and re-coupling the results over the initial-conditions.

Equations: $\partial_t c = Ac + Bc$, where the initial-conditions are $c(t^n) = c^n$.

Splitting-method of first order

\[
\begin{align*}
\partial_t c^* &= Ac^* \quad \text{with} \quad c^*(t^n) = c^n, \\
\partial_t c^{**} &= Bc^{**} \quad \text{with} \quad c^{**}(t^n) = c^*(t^{n+1}),
\end{align*}
\]

where the results of the methods are $c(t^{n+1}) = c^{**}(t^{n+1})$, and there are some splitting-errors for these methods.

Literature: [Strang 68], [Karlsen et al 2001].
Splitting-Errors of the Method

The error of the splitting-method of first order is

\[ \partial_t c = (B + A)c, \]
\[ \tilde{c} = \exp(\tau(B + A))c(t^n). \]

Local error for the decomposition and the full solution

\[ e(c) = \tilde{c}(t^n + \tau) - \exp(\tau B) \exp(\tau A)c(t^n), \]
\[ = \exp(\tau(B + A))c(t^n) - \exp(\tau B) \exp(\tau A)c(t^n), \]
\[ e(c)/\tau = \frac{1}{2} \tau(BA - AB)c(t^n) + O(\tau^2). \]

\( O(\tau) \) for A, B not commuting, otherwise one get exact results,

where \( \tau = t^{n+1} - t^n \), [Strang 68].
Higher order splitting-methods

Strang or Strang-Marchuk-Splitting, cf. [Marchuk 68, Strang68]

\[
\frac{\partial c^*(t)}{\partial t} = Ac^*(t), \text{ with } t^n \leq t \leq t^{n+1/2} \text{ and } c^*(t^n) = c_{sp}^n, \tag{6}
\]

\[
\frac{\partial c^{**}(t)}{\partial t} = Bc^{**}(t), \text{ with } t^n \leq t \leq t^{n+1}, \quad c^{**}(t^n) = c^*(t^{n+1/2}),
\]

\[
\frac{\partial c^{***}(t)}{\partial t} = Ac^{***}(t), \quad t^{n+1/2} \leq t \leq t^{n+1}, \quad c^{***}(t^{n+1/2}) = c^{**}(t^{n+1}),
\]

where \( t^{n+1/2} = t^n + 0.5\tau_n \) and the approximation on the next time level \( t^{n+1} \) is defined as \( c_{sp}^{n+1} = c^{***}(t^{n+1}) \).

The splitting error of the Strang splitting is

\[
\rho_n = \frac{1}{24}\tau_n^2([B, [B, A]] - 2[A, [A, B]]) c(t^n) + O(\tau_n^3). \tag{7}
\]

See, e.g.[Hundsdorfer, Verwer 2003].
Iterative splitting-Methods

\[
\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}(t), \text{ with } c_i(t^n) = c_{sp}^n, \tag{8}
\]

\[
\frac{\partial c_{i+1}(t)}{\partial t} = Ac_i(t) + Bc_{i+1}(t), \text{ with } c_{i+1}(t^n) = c_{sp}^n, \tag{9}
\]

where \(c_0(t)\) is any fixed function for each iteration. (Here, as before, \(c_{sp}^n\) 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 \(c_{sp}^{n+1} = c_{2m+1}(t^{n+1})\). (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 \(n\).)
Error for the Iterative splitting-method

**Theorem 9.1** The error for the splitting methods is given as:

\[
\|e_i\| = K\|B\|\tau_n\|e_{i-1}\| + O(\tau_n^2)
\]

(10)

and hence

\[
\|e_{2m+1}\| = K_m\|e_0\|\tau_n^{2m} + O(\tau_n^{2m+1}),
\]

(11)

(12)

where \(\tau_n\) 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 \(B\) and \(A\) and \(B\) are bounded, monotonic operators.

10 Generalisation: Waveform-Relaxation Method

We consider a nonlinear system of $n$ ordinary differential equations, i.e. after the spatial discretisation we get ODE's:

$$\frac{\partial c(t)}{\partial t} = f(t, y), \text{ with } c(0) = c_0, \ t \in [0, T], \quad (13)$$

where $T > 0$, $f : [0, T] \times \mathbb{R}^n \to \mathbb{R}^n$, $c_0 = (c_{1,0}, \ldots, c_{n,0})^t \in \mathbb{R}^n$ and the solution vector $c = (c_1, \ldots, c_n)^t \in \mathbb{R}^n$. 
Iterative Method: Wave-form-relaxation

\[
\frac{\partial c_1^\nu(t)}{\partial t} = f_1(t, y_1^\nu, y_2^\nu-1, \ldots, y_n^\nu-1), \quad (14)
\]
\[
\frac{\partial c_2^\nu(t)}{\partial t} = f_2(t, y_1^{\nu-1}, y_2^\nu, \ldots, y_n^{\nu-1}), \quad (15)
\]
\[
\ldots
\]
\[
\frac{\partial c_n^\nu(t)}{\partial t} = f_n(t, y_1^{\nu-1}, y_2^{\nu-1}, \ldots, y_n^\nu), \quad (16)
\]
with \( c_\nu(0) = c_0 \), \( t \in [0, T] \), \( (18) \).
Theory: Semi-group-theory

\[ \frac{\partial c^\nu(t)}{\partial t} + P c^\nu = Q c^{\nu-1} + f, \quad \text{with} \quad c^\nu(0) = c_0, \quad t \in [0, T], \quad (19) \]

Solution:

\[ c^\nu(t) = K c^{\nu-1}(t) + \phi, \quad (20) \]

\[ K c(t) = \int_0^t \exp((s - t)P) Q c(s) ds = \int_0^t k(t - s) c(s) ds, \quad (21) \]

\[ \phi(t) = \exp(-tP) c_0 + \int_0^t \exp((s - t)P) f(s) ds, \quad (22) \]

Theorem:

\[ \| c - c^\nu \|_\infty \leq \frac{(CT)^\nu}{\nu!} \| c - c_0 \|_\infty, \quad (23) \]

where \( \| k \|_\infty = C \) and \( k(t) = \exp(-tP)Q \)

Boundedness of \( P \) and \( Q \) important and \( c^{\nu-1}(t) \) near the local solution.
11 Domain-Decomposition-Methods for a system of parabolic equations

Idea for the overlapping Schwarz wave form relaxation for the convection-diffusion equation.

\[ u_t = D u_{xx} - \nu u_x - \lambda u , \tag{24} \]

defined over the domain \( \Omega = [0, L] \) for \( t = [t_0, t_{\text{end}}] \), with the following initial and boundary conditions

\[ u(0, t) = f_1(t), \quad u(L, t) = f_2(t), \quad u(x, t_0) = u_0 . \]

We decouple the domain \( \Omega \) in two overlapping sub-domains \( \Omega_1 = [0, L_2] \) and \( \Omega_2 = [L_1, L] \), where \( L_1 < L_2 \) and \( \Omega_1 \cap \Omega_2 = [L_1, L_2] \) is the overlapping region for \( \Omega_1 \) and \( \Omega_2 \).
The application in 2 different domains, we deal with 2 equations:

\[
\begin{align*}
  v_t &= Dv_{xx} - \nu v_x - \lambda v \text{ over } \Omega_1, \\
  v(0, t) &= f_1(t), \\
  v(L_2, t) &= w(L_2, t), \\
  v(x, t_0) &= u_0, \\
  w_t &= Dw_{xx} - \nu w_x - \lambda w \text{ over } \Omega_2, \\
  w(L_1, t) &= v(L_1, t), \\
  w(L, t) &= f_2(t), \\
  w(x, t_0) &= u_0,
\end{align*}
\]

(25)

where \( v(x, t) = u(x, t)|_{\Omega_1} \) and \( w(x, t) = u(x, t)|_{\Omega_2} \).
Theorem 11.1  Let $e^k = u^k - v^k$ and $d^k = u^k - w^k$ be the error from the solution to the subproblems (25) and (26) by Schwarz waveform relaxation over $\Omega_1$ and $\Omega_2$, respectively, then

$$|e^{k+2}(x, t)| \leq \gamma \|e^k(L_1, \cdot)\|_\infty,$$

and

$$|d^{k+2}(x, t)| \leq \gamma \|d^k(L_2, \cdot)\|_\infty,$$

for all $(x, t)$, where $\beta = \frac{\sqrt{\nu^2 + 4D\lambda}}{2D}$,

$$\|e^1(L_1, \cdot)\|_\infty \leq \max_{t \in [t_0, t_{\text{end}}]} \{ f_1(\cdot), f_2(\cdot), u_0(L_1) \},$$

$$\|d^1(L_2, \cdot)\|_\infty \leq \max_{t \in [t_0, t_{\text{end}}]} \{ f_1(\cdot), f_2(\cdot), u_0(L_2) \},$$

and

$$\gamma = \frac{\sinh(\beta L_1) \sinh(\beta (L - L_2))}{\sinh(\beta L_2) \sinh(\beta (L - L_1))}.$$
12 Discretisation-Methods

Based on Standard Methods we modify:

- Finite Volume Methods (Box-Methods with FBMC, Characteristic-Methods)
- Discontinuous Galerkin Methods (Embed of analytical local methods)
- Improved Finite-Element-Methods (near-field, finite-element-method and far-field, Greens-function-method)
### 13 Advanced Discretisation-Methods, integration of decomposing methods

<table>
<thead>
<tr>
<th>Discretisation Method</th>
<th>Modification for the method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finite Volumes</td>
<td>Reconstruction Method</td>
</tr>
<tr>
<td>Finite Element</td>
<td>Enriched Methods (e.g. Bubble Functions)</td>
</tr>
<tr>
<td>Discontinuous Galerkin</td>
<td>Embedded Test-functions (e.g. one-dimensional solutions)</td>
</tr>
</tbody>
</table>

Table 1: Modifications for the Standard Methods
14 Motivation for the discretisation methods for the Parabolic and Hyperbolic Differential-Equations

1.) Characteristic methods (Transport and reaction exact):
Test-functions (linear or constant) are exact transported. Only approximation error for the initial condition and splitting error in multi-dimensions.

2.) Locally improved test-functions
New improved test-space for the Finite Volume or DG-methods, locally exact solutions.

3.) Locally improved trial-functions to improve the discretisation of critical terms. Idea skip the critical terms via analytical solutions.
15 Discretization-methods based on Voronoi-Boxes

- Local Mass-conservation, Simple test-functions (box-functions).
- Un-structured Grids (adaptive grids), dual mesh.

\[ T^e \text{ Elements, } e = 1, \ldots, E, \text{ number of elements.} \]

\[ \Omega_j \text{ dual cells, } j = 1, \ldots, N, \text{ number of nodes.} \]
16 Improved discretisation methods via exact transport and reaction on the Characteristics

The scalar equation is given by:

$$\partial_t R c + \nabla \cdot v c = 0.0,$$

where the initial-conditions are $c(x, t^0) = c^0(x)$.

The spatial-integration plus the Theorem of Gauss for the derivatives:

$$\int_{\Omega_j} \partial_t (R c) \, dx = - \int_{\Omega_j} \nabla \cdot (v c) \, dx = - \int_{\Gamma_j} n \cdot (v c) \, d\gamma,$$

where $\Omega_j$ is the j-th cell and $v_{jk} = n_{jk} \cdot \int_{\Gamma_{jk}} v(\gamma) \, d\gamma$.

$$|\Omega_j|(R(c_j^{n+1}) - R(c_j^n)) = -\tau^n \sum_{k \in \text{out}(j)} v_{jk} \tilde{c}_{jk}^n + \tau^n \sum_{l \in \text{in}(j)} v_{lj} \tilde{c}_{lj}^n.$$
The discretization-scheme with the mass-notation is:

\[
m_j^{n+1} - m_j^n = - \sum_{k \in out(j)} m_{jk}^n + \sum_{l \in in(j)} m_{lj}^n ,
\]

where:

\[
m_j^n = V_j \ R \ c_j(t^n) , \quad m_{jk}^n = \tau \ \tilde{c}_{jk}^n v_{jk} ,
\]

with the limitation to fulfill the monotonicity (local min-max-property).

We use the reconstruction of the linear test-function: \( c_{jk}^n = c_j^n + \nabla c_j^n (x_{jk} - x_j) \)

Limiters (Slope and Flux-Limiter):

\[
\min_{k \in in(i)} \{ c_i^n, c_k^n \} \leq c_{jk}^n \leq \max_{k \in in(i)} \{ c_i^n, c_k^n \} , \quad j \in out(i) , \quad \text{with limited value } \tilde{c}_{jk}^n ,
\]

\[
\tilde{c}_{jk}^n = \tilde{c}_{jk}^n + \frac{\tau}{\tau_j} (c_j^n - \tilde{c}_{jk}^n) , \quad \tau_j = \frac{V_j}{\nu_j} ,
\]

\[
\nu_j = \sum_{k \in out(j)} \nu_{jk} , \quad \nu_{jk} = n_{jk} \cdot \int_{\Gamma_{jk}} v(\gamma) \ d\gamma .
\]
Higher order FV-Discretisation by $P^2$ lagrangian elements

Idea: $P^2$-elements with the dual cells:

Spaces: Trial-Space: $P^2$-elements, Test-Space: $P^0$-elements
17 Discussion of the effectivity, Parallelisation and Implementation

- All decoupling methods are parallelisable and could be simple implemented.
- The decoupling methods are therefore effective and fast.
- For strong coupling the structure could be destroyed.
- To decouple the equations one could use physical characteristics of the equation as: Neumann-, Courant- and Peclet-Number for the convection-diffusion equation.
- Lower order initialisation methods are important to stabilise the methods, and to start with a value $c_{\nu} \approx c$.
- Higher order methods could be used while the local solutions are improved (hierarchy of lower-higher order solvers).
18 Calculation of a potential damage case

3 dim. domain $6000[m] \times 1500[m]$ with groundwater-flow, Project-partner: GRS
The decay chain of a realistic potential damage events

\[ Pu-244 \rightarrow Pu-240 \rightarrow U-236 \rightarrow Th-232 \rightarrow Ra-228 \]

\[ Cm-244 \rightarrow Pu-240 \]

\[ U-232 \]

\[ Pu-241 \rightarrow Am-241 \rightarrow Np-237 \rightarrow U-233 \rightarrow Th-229 \]

\[ Cm-246 \rightarrow Pu-242 \rightarrow U-238 \rightarrow U-234 \rightarrow Th-230 \rightarrow \]

\[ Ra-226 \rightarrow Pb-210 \]

\[ Am-242 \rightarrow Pu-238 \rightarrow U-234 \]

\[ Am-243 \rightarrow Pu-239 \rightarrow U-235 \rightarrow Pa-231 \rightarrow Ac-227 \]

Uranium is very dangerous because it is few retarded and decayed very slow.
Concentration of U-236 in the time $t = 100 \ [a]$.

(Visualized with the program Grape (University Freiburg, Germany).)
Concentration of von U-236 in the time $t = 10000 \ [a]$. 
20 Project: Crystal-Growth

Content of software-tool-box WIAS-HiTNIHS:

- Transient simulation tool for the temperature evolution
- Axisymmetric technical system reduced to a 2d problem
- Modelling induction-heating by solving a Maxwell-equation
- Heat transfer by radiation through cavities
- Temperature-dependent laws of thermal and electrical conductivity and for the material parameters
- Anisotropy of the insulation-materials.
Model: Production of SiC by physical vapor transport

- Inside a heated graphite crucible, polycrystalline SiC source powder sublimates at temperatures between 2000 K and 3000 K.
- Diffusion of the gaseous SiC through the inert gas Ar from the source powder to the seed.
- Crystallization on the cooled seed leads to the growth of a single bulk crystal.

**Fig:** Setup of growth apparatus according to Pons et al. (1999) inserted in a tube.
**Anisotropic heat flux**

The insulation consists of graphite felt, having an anisotropic structure.

We deal with a heat flux $\vec{q}$ of the form

$$
\vec{q} = \vec{q}(r, \phi) = -\kappa(T) \begin{pmatrix}
\alpha_r & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & \alpha_z
\end{pmatrix} \text{grad } T \text{ is used, where}
$$

- $(r, \phi, z)$ are the cylindrical polar coordinates,
- $T = T(r, z)$ is the temperature,
- $\kappa$ is a temperature dependent thermal conductivity,
- $\alpha_r, \alpha_z$ are given positive constants.
Isotropic and anisotropic insulation
21 Application of the Black-Box-Solver

Multi-physical problem:
Heat-transport, gas-transport, reaction and growth-processes.

Multi-dimensional problem:
Material regions, with different parameters

Multi-scaling problem:
Anistropic effects, reaction-processes with different scales

Idea: Using software-codes for different effect, e.g. heat-transfer (WIAS-HiTNIHS-code), gas-transport (Navier-Stokes-code) and using Black-Box-Solver for the different interface-problems.
22 Conclusions

- Physical Operator-Splitting with respect to the physical behaviour (decoupling of equation-parts).

- Waveform-Relaxation method as an iterative solver for iterative Operator-Splitting methods

- Higher order spatial discretisation methods correspond with order of the time-discretisation (embedding higher order time-discretisation methods, e.g. BDF-methods) order increase.

- Applications in material problems, e.g. coupling of different micro- and macro-structures.

- Black-Box solver for the crystal-growth (coupling further physical phenomenons, e.g. gas-transport, reaction-model and growth of the crystal)