On iterative solvers combined with projected Newton methods for reacting flow problems

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Outline

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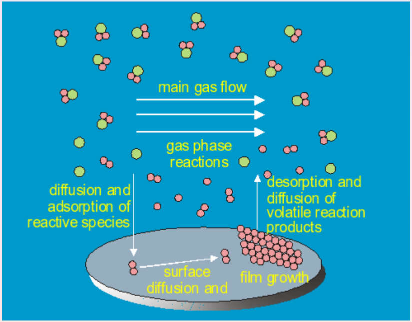
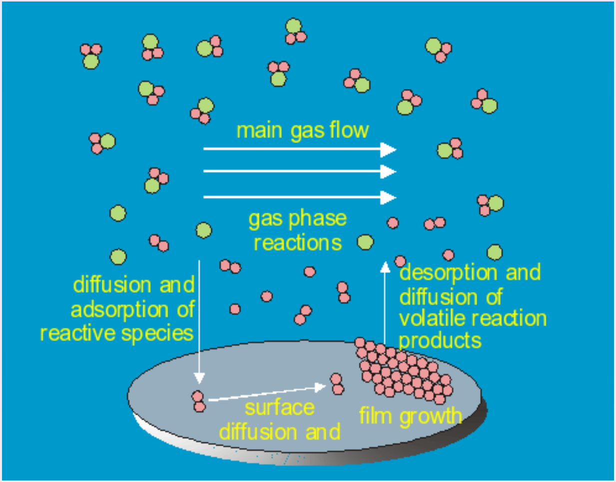
Chemical Vapor Deposition

- Transforms gaseous molecules into high purity, high performance solid materials
- Thin film, or powder
- Thermal energy drives (gas phase and surface) reactions

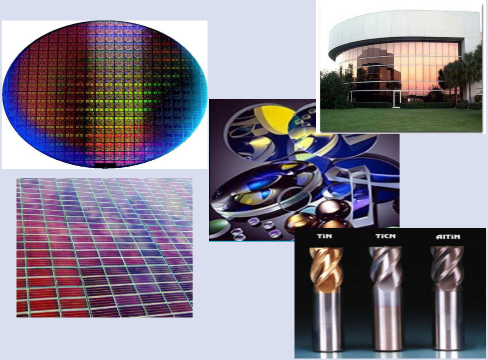


Chemical Vapor Deposition



Chemical Vapor Deposition

Applications



- Semiconductors
- Solar cells
- Optical, mechanical and decorative coatings

Transport Model for CVD

Mathematical Model

Conservation of:

- Total mass: Continuity equation
- Momentum: Navier-Stokes equations
- Energy: Transport eqn for thermal energy

Closed by:

- Ideal gas law

- Transport of species i

$$\frac{\partial(\rho\omega)}{\partial t} = \nabla \cdot (\rho v \omega) + \nabla \cdot \mathbf{j}_i + m \sum_{k=1}^{\#\text{reactions}} \nu_k R_k^G$$

Transport Model for CVD

Reaction Rate

- Net molar gas phase reaction rate

$$R_i^G = A_i \cdot T^{\beta_i} \cdot e^{-\frac{E_i}{RT}} \cdot F(P, T, \omega_1, \ldots, \omega_i, \ldots, \omega_N)$$

- Surface reaction rate

$$R_i^S = \frac{\gamma_i}{1 + \gamma_i/2} \cdot G(P, T, \omega_i)$$

- Time constants of slowest and fastest reactions differ orders of magnitude
- Stiff nonlinear system of species equations

Numerical Methods

Goal

- Time accurate transient solution
- Start up & shut down cycli

Properties

- Stiff Problem $\longrightarrow$ Stable Time Integration
- Positivity (= preservation of non-negativity):
  Negative Species can blow up of the solution
- Efficiency / Robustness
- Method of Lines approach

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Positivity

Mass fractions

A natural property for mass fractions is their non-negativity

Positivity of mass fractions should hold for . . .

1. Model equations
2. Spatial discretization: Hybrid scheme
   Introduces locally first order upwinding
3. Time integration
4. Iterative solvers:
   (Non)linear solver

Positivity for ODE systems

Euler Backward

- $w_{n+1} - w_n = \tau F(t_{n+1}, w_{n+1})$
- Unconditionally stable (A-stable/ stiffly stable)

Theorem (Hundsdorfer, 1996)

Euler Backward is positive for any step size τ

Theorem (Bolley and Crouzeix, 1970)

Any unconditionally positive time integration is at most first order accurate

Positivity for ODE systems

With respect to time integration we conclude . . .

- Restrict time integration to EB
- How to deal with huge nonlinear systems?
- How to maintain the unconditional positivity within nonlinear solver?

Nonlinear Solvers

Globalized Inexact Newton to solve $F(x) = 0$

Let x_0 be given.
FOR $k = 1, 2, \ldots$ until 'convergence'
Find some $\eta_k \in [0, 1)$ and s_k that satisfy

$$\|F(x_k) + F'(x_k)s_k\| \leq \eta_k \|F(x_k)\|.$$

WHILE $\|F(x_k + s_k)\| > (1 - \alpha(1 - \eta_k))\|F(x_k)\|$ **DO**
Choose $\lambda \in [\lambda_{\min}, \lambda_{\max}]$
Set $s_k \leftarrow \lambda s_k$ and $\eta_k \leftarrow 1 - \lambda(1 - \eta_k)$
ENDWHILE
Set $x_{k+1} = x_k + s_k$.
ENDFOR

Nonlinear Solvers

Globalized Inexact Projected Newton to solve $F(x) = 0$

Let x_0 be given.
FOR $k = 1, 2, \ldots$ until 'convergence'
Find some $\eta_k \in [0, 1)$ and s_k that satisfy

$$\|F(x_k) + F'(x_k)s_k\| \leq \eta_k \|F(x_k)\|.$$

WHILE $\|F(\mathcal{P}(x_k + s_k))\| > (1 - \alpha(1 - \eta_k))\|F(x_k)\|$ **DO**
Choose $\lambda \in [\lambda_{\min}, \lambda_{\max}]$
Set $s_k \leftarrow \lambda s_k$ and $\eta_k \leftarrow 1 - \lambda(1 - \eta_k)$
ENDWHILE
Set $x_{k+1} = \mathcal{P}(x_k + s_k)$.
ENDFOR

Nonlinear Solvers

Note that

- Forcing term η_k in

$$\|F(x_k) + F'(x_k)s_k\| \leq \eta_k \|F(x_k)\|.$$

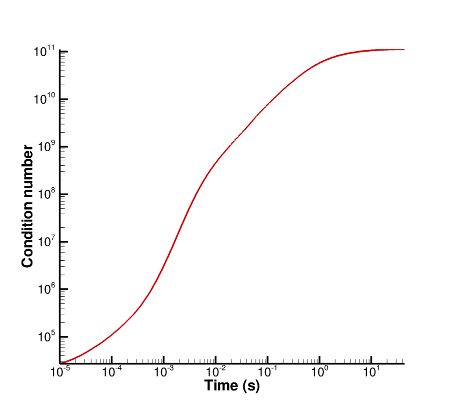
  is a certain accuracy in solving $F'(x_k)s_k = -F(x_k)$
- How to choose η_k?
- η_k too small $\Rightarrow$ oversolving
- Ideal: Based on residual norms as

$$\eta_k = \gamma \frac{\|F(x_k)\|^2}{\|F(x_{k-1})\|^2}$$

Preconditioned Krylov solvers

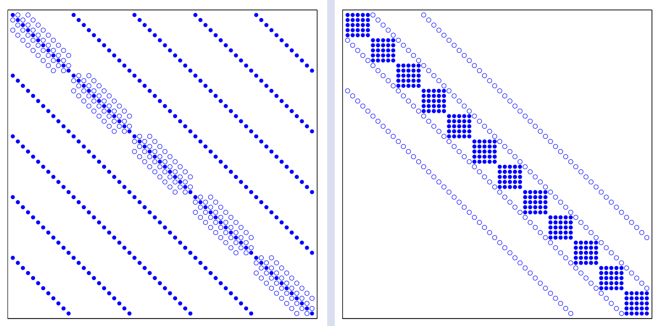
Properties

- Huge condition numbers due to chemistry terms



Preconditioned Krylov solvers

Lexicographic ordering (left) and Alternate blocking per grid point(right)



Preconditioned Krylov solvers

Iterative Linear Solver

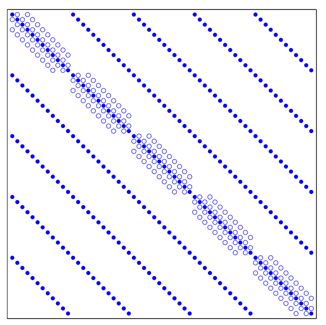
- Right preconditioned BiCGStab
- 'Heavy' chemistry terms $\rightarrow$ diagonal blocks
- Incomplete Factorization: ILU(0)

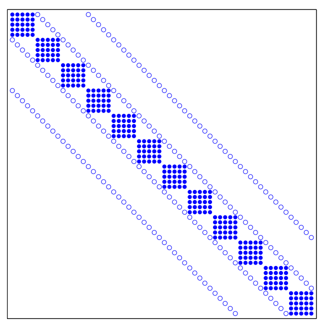
Number of	lexico graphic	alternate blocking per gridpoint
F	220	197
Newton iters	124	111
Linesearch	12	7
Rej. time steps	0	0
Acc. time steps	36	36
CPU Time	400	300
linear iters	444	346

Preconditioned Krylov solvers

Preconditioners: Lumping

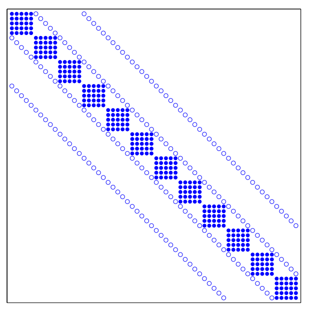
Important: Lumping per species





Preconditioned Krylov solvers

Preconditioners: Block Diagonal



- ‘natural’ blocking over species
- series of uncoupled systems $\longrightarrow$ LU factorization per subsystem

Preconditioned Krylov solvers

Preconditioners: Block D-ILU

Put $D_{ii} = A_{ii}$ for all $i = 1, \ldots, n$

FOR $i = 2, \ldots, n$

  IF $\mod(i, nr) \neq 0$ **THEN**

    $D_{i+1,i+1} = D_{i+1,i+1} - A_{i+1,i} D_{ii}^{-1} A_{i,i+1}$

  ENDIF

  IF $i + nr \leq s \cdot n$ **THEN**

    $D_{i+nr,i+nr} = D_{i+nr,i+nr} - A_{i+nr,i} D_{ii}^{-1} A_{i,i+nr}$

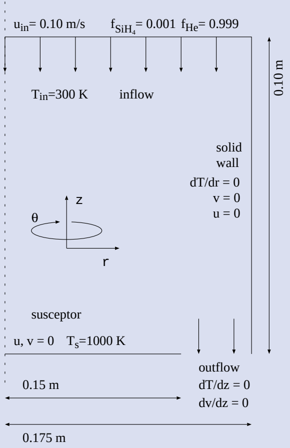
  ENDIF

ENDFOR

- Computation of $D_{ii}^{-1} A_{i,i+1}$
- Gauss-Jordan decomposition of D_{ii}

Kleijn's Benchmark Problem

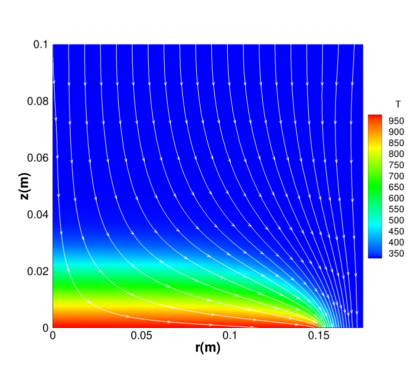
Computational Domain



- Axisymmetric
- 0.1 mole% SiH_4 at the inflow
- Rest is carrier gas helium He
- Susceptor does not rotate

Kleijn’s Benchmark Problem

Computational Domain



- Grid sizes: 35×32 up to 70×82 grid points
- Temperature:
  Inflow 300 K
  Susceptor 1000 K
- Uniform velocity at inflow

Kleijn's Benchmark Problem

Chemistry Model: 16 species, 26 reactions [1]

- Above heated wafer SiH_4 decomposes into SiH_2 and H_2
- Chain of 25 homogeneous gas phase reactions
- Including the carrier gas the gas mixture contains 17 species, of which 14 contain silicon atoms
- Irreversible surface reactions at the susceptor leads to deposition of solid silicon

[1] M.E. Coltrin, R.J. Kee and G.H. Evans, A Mathematical Model of the Fluid Mechanics and Gas-Phase Chemistry in a Rotating Chemical Vapor Deposition Reactor, J. Electrochem. Soc., 136, (1989)

Numerical Results

Integration statistics: 35 $\times$ 32 grid

	ILU(0)	Lumped Jac	block DILU	block diag	direct solver
Newton	108 (101)	149 (127)	104 (93)	1,379 (125)	94
linesearch	9 (6)	16	6 (4)	7 (16)	11
Negative	1 (0)	3 (0)	2 (0)	403 (0)	1
Acc. steps	38 (36)	41 (36)	39 (36)	724 (36)	38
lin iters	848 (825)	7,927 (5,819)	838 (718)	13,371 (6,275)	
CPU	300 (270)	530 (410)	320 (270)	3,610 (450)	6,500

- Black: Globalized Inexact Newton
- Red: Globalized Inexact Projected Newton

Numerical Results

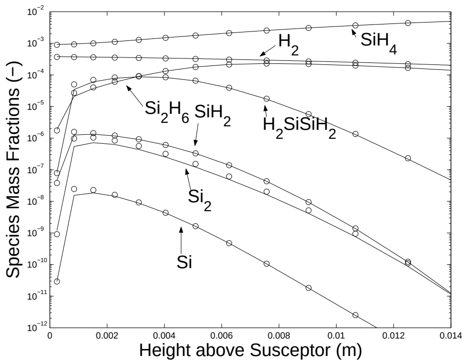
Integration statistics: 70 $\times$ 82 grid

Preconditioner	ILU(0)	block D-ILU
Newton iter	395 (351)	299 (306)
Negative	3(0)	0
Acc time step	41 (37)	37
line search	136 (128)	101 (96)
lin iters	11,100 (8,895)	2,144 (2,290)
CPU time (sec)	5,420 (6,000)	4,175 (4,350)

- Black: Globalized Inexact Newton
- Red: Globalized Inexact Projected Newton
- Direct solver is not feasable

Kleijn's Benchmark Problem

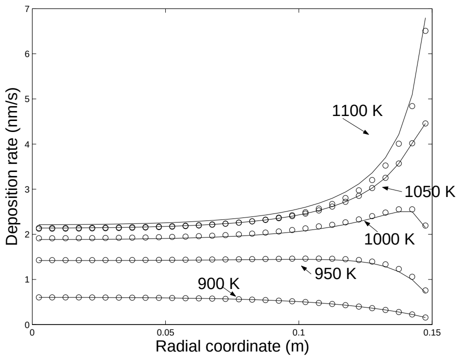
Validation: Species mass fraction along the symmetry axis



- solid: Kleijn's solutions
- circles: our solutions

Kleijn’s Benchmark Problem

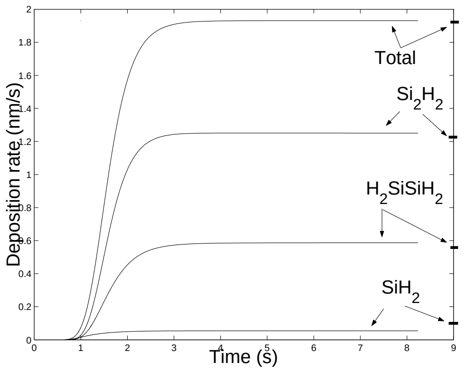
Validation: Radial profiles of total steady state deposition rate



- wafer temperature from 900 K up to 1100 K
- solid: Kleijn’s solutions
- circles: our solutions

Kleijn's Benchmark Problem

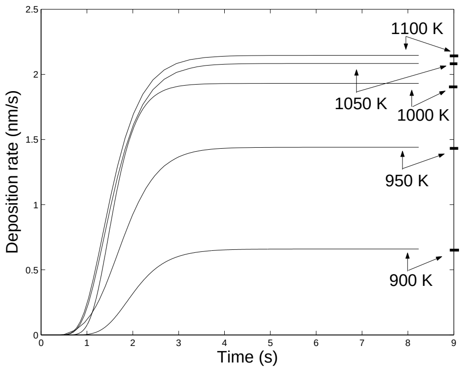
Transient behavior of deposition rates



- along symmetry axis
- wafer 1000 K

Kleijn's Benchmark Problem

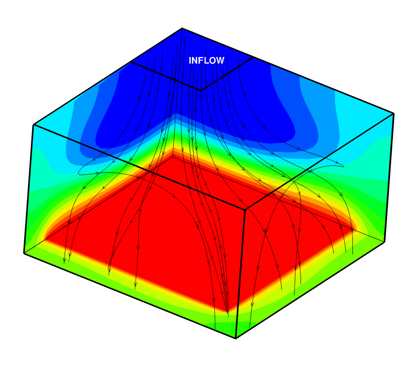
Transient behavior of deposition rates



- along symmetry axis
- wafer temperatures from 900 up to 1100 K

3D Results on Kleijn's Benchmark Problem

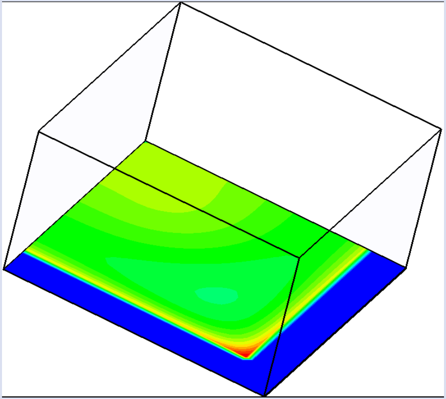
Computational Domain



- Grid sizes: $35 \times 32 \times 35$
- Temperature:
  Inflow 300 K
  Susceptor 1000 K
- Uniform velocity at inflow

3D Results on Kleijn's Benchmark Problem

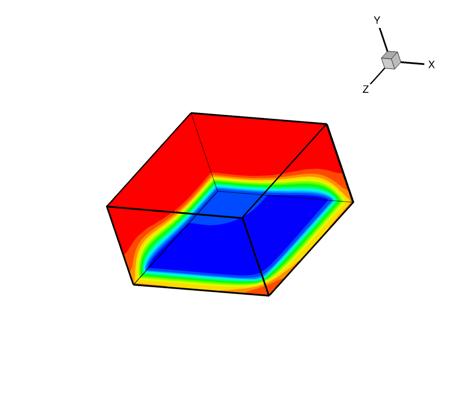
Total deposition rate



- On centerline: total deposition rate of 2.41 nm/s
- Compare with 2D results: 2.43 nm/s along symmetry axis

3D Results on Kleijn's Benchmark Problem

Concentration profile SiH_4



Numerical Results

Integration statistics: 35 $\times$ 32 $\times$ 35 grid

	ILU(0)	Lumped Jac	block DILU	block diag
Newton	239	332	156	327
linesearch	51	31	20	29
Newt Diver	3	0	0	0
Acc. time step	44	43	43	43
lin iters	3,196	17,472	2,481	18,392
CPU	20,100	28,000	17,500	29,000

- Without Projected Newton not feasible

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Conclusions and Future Research

Conclusions

- Globalized Inexact Projected Newton maintains the unconditional positivity of Euler Backward
- Alternate blocking per grid point is more effective
- Easy preconditioners are effective for 2D and 3D problems
- Chemistry source terms should be in the preconditioner

Future Research

- More realistic chemistry/surface chemistry models
- Steady state solver

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References and Contact Information

References

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- "—", *Comparison of ODE Methods for Laminar Reacting Gas Flow Simulations*, Num. Meth. Part. Diff. Eq., to appear, (2008)
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References and Contact Information

Contact Information

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