Fast Solvers for Linear Systems on the GPU

GPU Technology Conference (GTC), San Jose, March 23-27, 2014

Session S4299

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March 25th, 2014, c.vuik@tudelft.nl, GTC S4299

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Main question:

Can ILU preconditioners be combined with GPU's?

1. Problem description: ship simulator

Linearized Variational Boussinesq for interactive waves:

$$\frac{\partial \zeta}{\partial t} + \nabla \cdot (\zeta \mathbf{U} + h\nabla\varphi - h\mathcal{D}\nabla\psi) = 0, \tag{1a}$$

$$\frac{\partial \varphi}{\partial t} + \mathbf{U} \cdot \nabla\varphi + g\zeta = -P_s, \tag{1b}$$

$$\mathcal{M}\psi + \nabla \cdot (h\mathcal{D}\nabla\varphi - \mathcal{N}\nabla\psi) = 0. \tag{1c}$$

After discretization (FVM for space, Leapfrog for time):

$$A\vec{\psi} = \mathbf{b}, \tag{2}$$

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = L\mathbf{q} + \mathbf{f}. \tag{3}$$

Properties of the system matrix

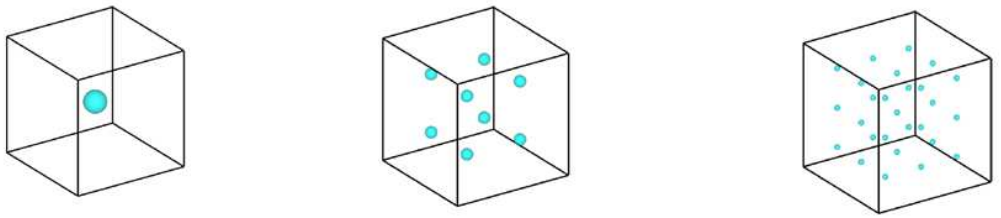
The system matrix A is given by a 5-point stencil:

$$\begin{bmatrix} 0 & -\frac{\Delta x}{\Delta y}\overline{\mathcal{N}_N} & 0 \\ -\frac{\Delta y}{\Delta x}\overline{\mathcal{N}_W} & \frac{\Delta x}{\Delta y}\overline{\mathcal{N}_N} + \frac{\Delta y}{\Delta x}\overline{\mathcal{N}_E} + \Delta x \Delta y \mathcal{M}_C + \frac{\Delta x}{\Delta y}\overline{\mathcal{N}_S} + \frac{\Delta y}{\Delta x}\overline{\mathcal{N}_W} & -\frac{\Delta y}{\Delta x}\overline{\mathcal{N}_E} \\ 0 & -\frac{\Delta x}{\Delta y}\overline{\mathcal{N}_S} & 0 \end{bmatrix}.$$

Matrix A is:

- real-valued, sparse (5-point, pentadiagonal)
- diagonally dominant (not very strong for small mesh sizes)
- symmetric positive definite (SPD)
- quite large

Problem Description: Bubbly Flow



Mass-Conserving Level-Set method for Navier Stokes

$$-\nabla.(\frac{1}{\rho(x)}\nabla p(x)) = f(x),\ x \in \Omega \tag{4}$$

$$\frac{\partial}{\partial n}p(x) = 0,\ x \in \partial\Omega \tag{5}$$

- Pressure-Correction equation is discretized to $Ax = b$.
- Most time consuming part is the solution of this SPSD system

2. Preconditioners: RRB

The RRB-solver:

- is a PCG-type solver (Preconditioned Conjugate Gradient)
- uses as preconditioner: the RRB preconditioner

RRB stands for “Repeated Red-Black”.

The RRB preconditioner determines an incomplete factorization:

$$A = LDL^T + R \quad \Longrightarrow \quad M = LDL^T \approx A$$

Preconditioners: RRB

As the name RRB reveals: multiple levels

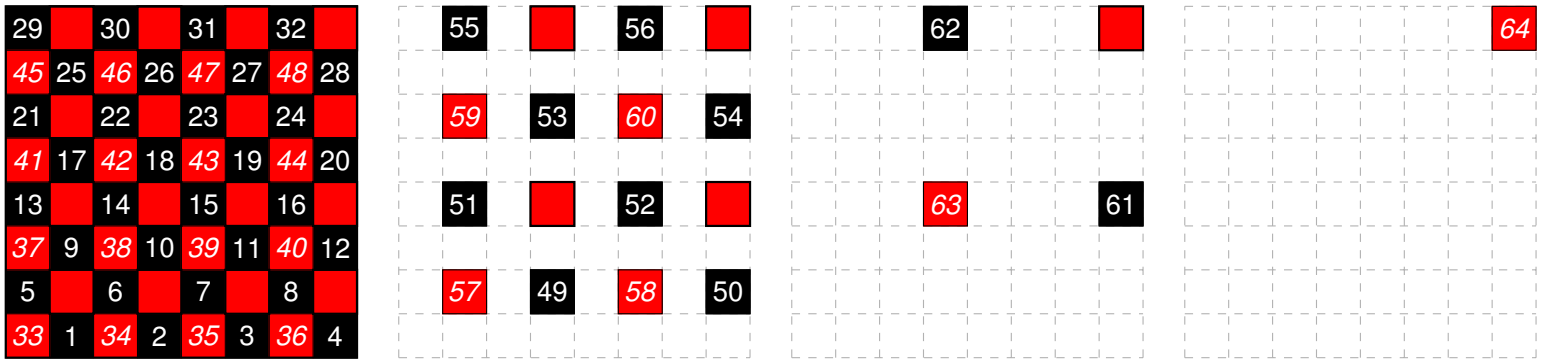
Therefore the RRB-solver has good scaling behaviour (Multigrid)

Method of choice because:

- shown to be robust for all of MARIN's test problems
- solved all test problems up to 1.5 million nodes within 7 iterations(!)

Special ordering (1)

An 8×8 example of the RRB-numbering process



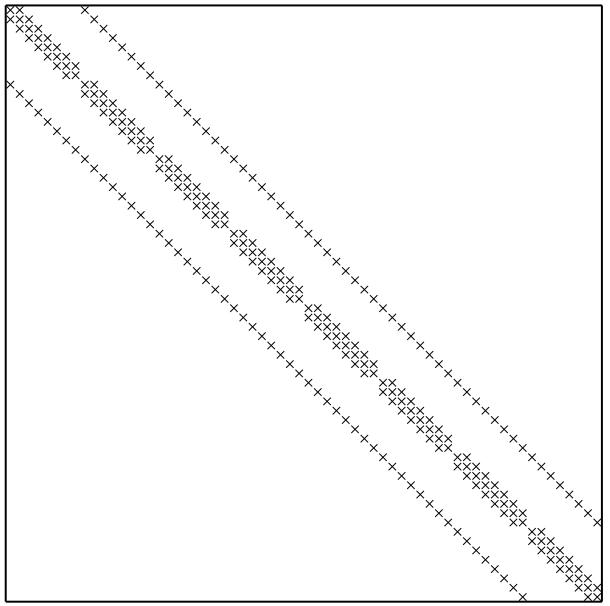
(1) (2) (3) (4)

All levels combined:

29	55	30	62	31	56	32	64
45	25	46	26	47	27	48	28
21	59	22	53	23	60	24	54
41	17	42	18	43	19	44	20
13	51	14	63	15	52	16	61
37	9	38	10	39	11	40	12
5	57	6	49	7	58	8	50
33	1	34	2	35	3	36	4

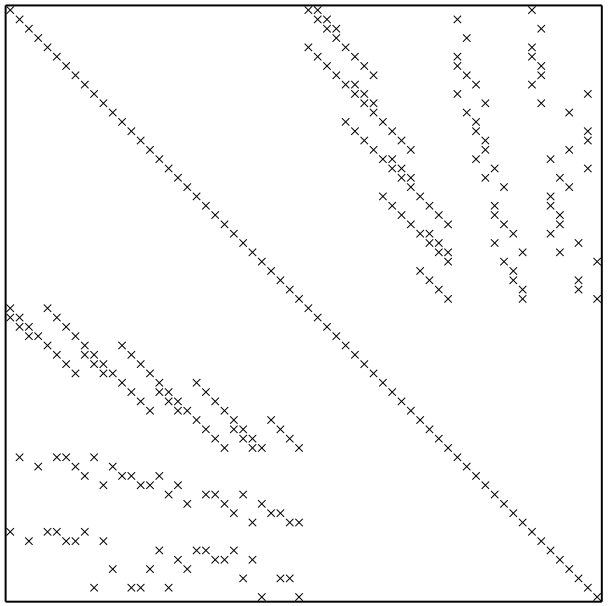
Special ordering (2)

Effect on sparsity pattern of matrix A:



Lexicographic

becomes

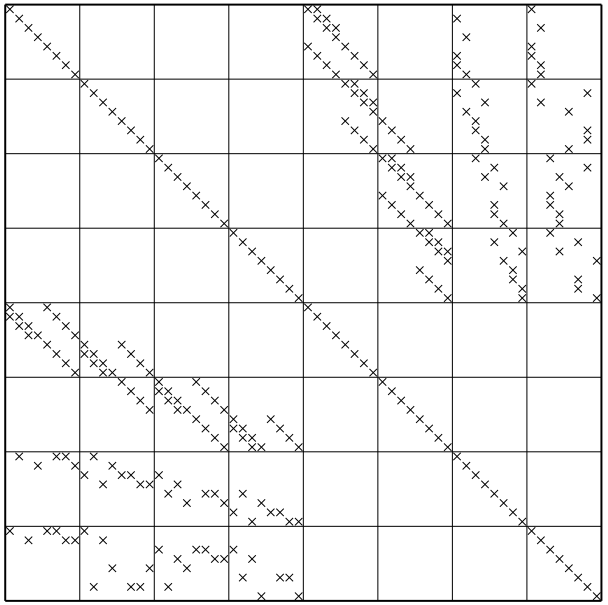


RRB-numbering

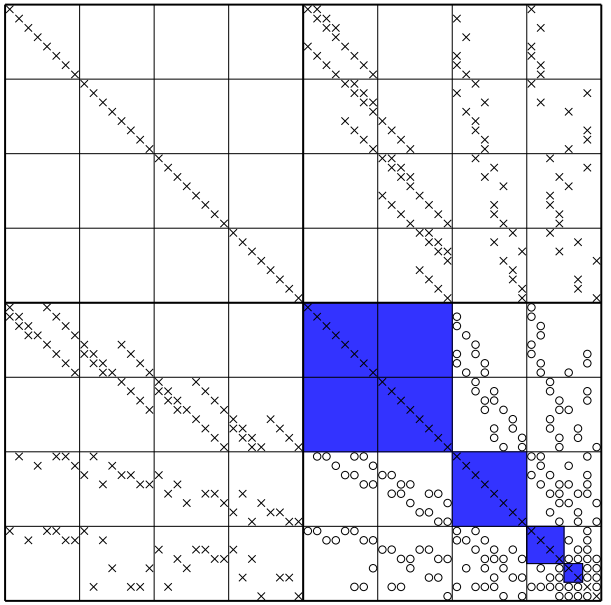
Special ordering (3)

Sparsity pattern of matrix A versus $L + D + L^T$

(recall preconditioner $M = LDL^T$)



becomes



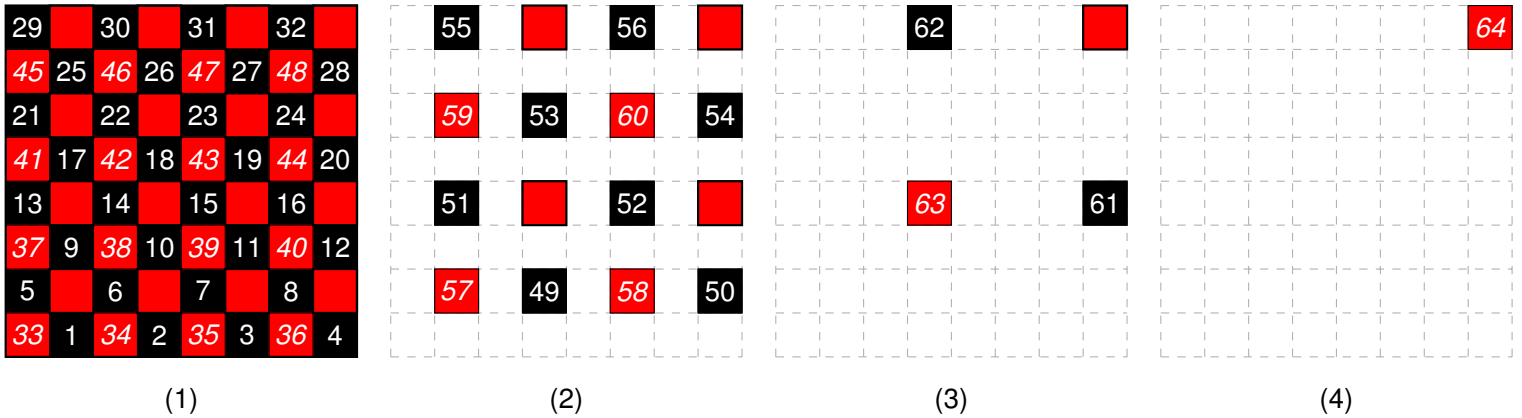
In the blue shaded areas fill-in has been dropped (lumping)

CUDA implementation (1)

Besides the typical Multigrid issues such as idle cores on the coarsest levels, in CUDA the main problem was getting “coalesced memory transfers”.

Why is that?

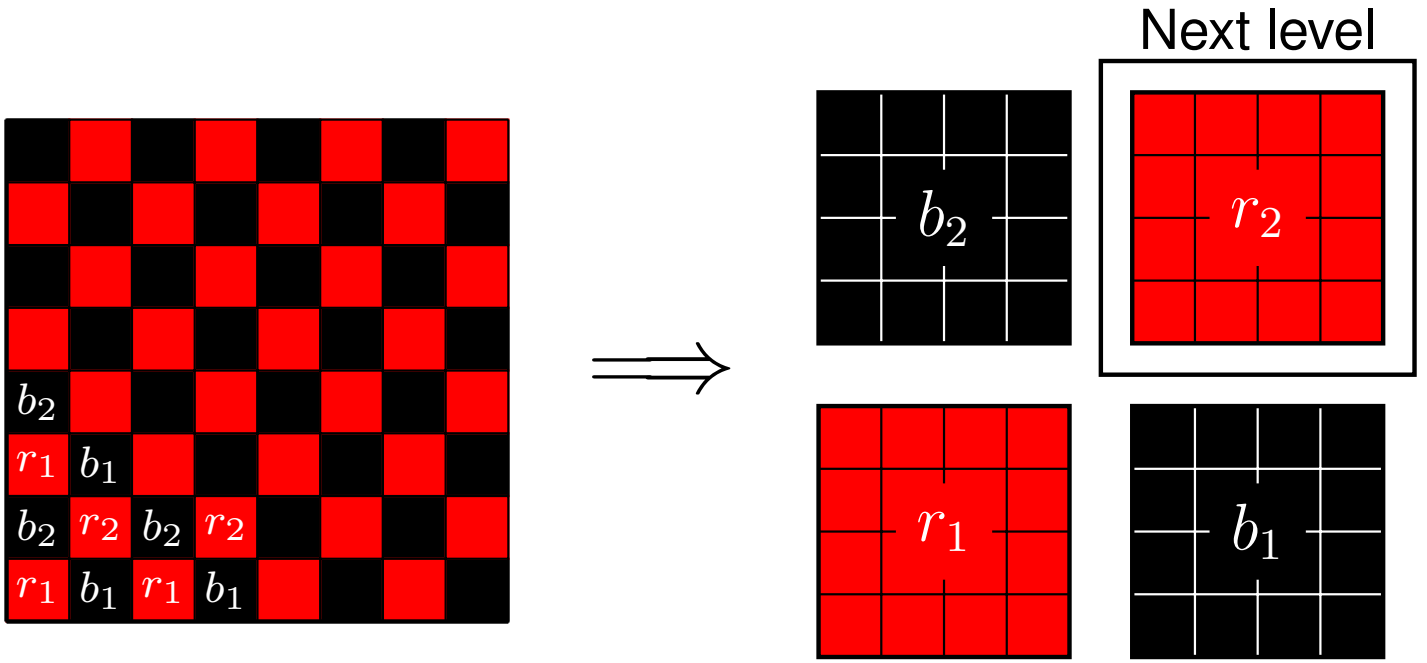
Recall the RRB-numbering: the number of nodes becomes 4$\times$ smaller on every next level:



CUDA implementation (2)

New storage scheme: $r_1/r_2/b_1/b_2$

Nodes are divided into four groups:



Preconditioners: TNS

Truncated Neumann Series Preconditioning[a],[b]

$$M^{-1} = K^T D^{-1} K, \text{ where } K = (I - LD^{-1} + (LD^{-1})^2 + \cdots)$$

L is the strictly lower triangular of A, and D=diag(A).

1. More terms give better approximation.
2. In general the series converges if $\| LD^{-1} \|_\infty < 1$.
3. As much parallelism as Sparse Matrix Vector Product.

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[a] A vectorizable variant of some ICCG methods. Henk A. van der Vorst. SIAM Journal of Scientific Computing. Vol. 3 No. 3 September 1982.

[b] Approximating the Inverse of a Matrix for use in Iterative Algorithms on Vector Processors. P.F. Dubois. Computing (22) 1979.

Preconditioners: Deflation

Removes small eigenvalues from the spectrum of $M^{-1}A$.

The linear system $Ax = b$ can be solved by the splitting,

$$x = (I - P^T)x + P^T x \text{ where } P = I - AQ. \tag{6}$$

$$\Leftrightarrow Pb = PA\hat{x}. \tag{7}$$

$Q = ZE^{-1}Z^T$, $E = Z^T AZ$.

$Em = a1$ is the coarse system

Z is an approximation of the 'bad' eigenvectors of $M^{-1}A$.

For our experiments Z consists of piecewise constant vectors.

Preconditioners: Deflation

Operations involved in deflation[a] [b].

- $a1 = Z^T p$.
- $m = E^{-1} a1$.
- $a2 = AZm$.
- $\hat{w} = p - a2$.

where, $E = Z^T AZ$ is the Galerkin Matrix and Z is the matrix of deflation vectors.

[a] Efficient deflation methods applied to 3-D bubbly flow problems. J.M. Tang, C. Vuik Elec. Trans. Numer. Anal. 2007.

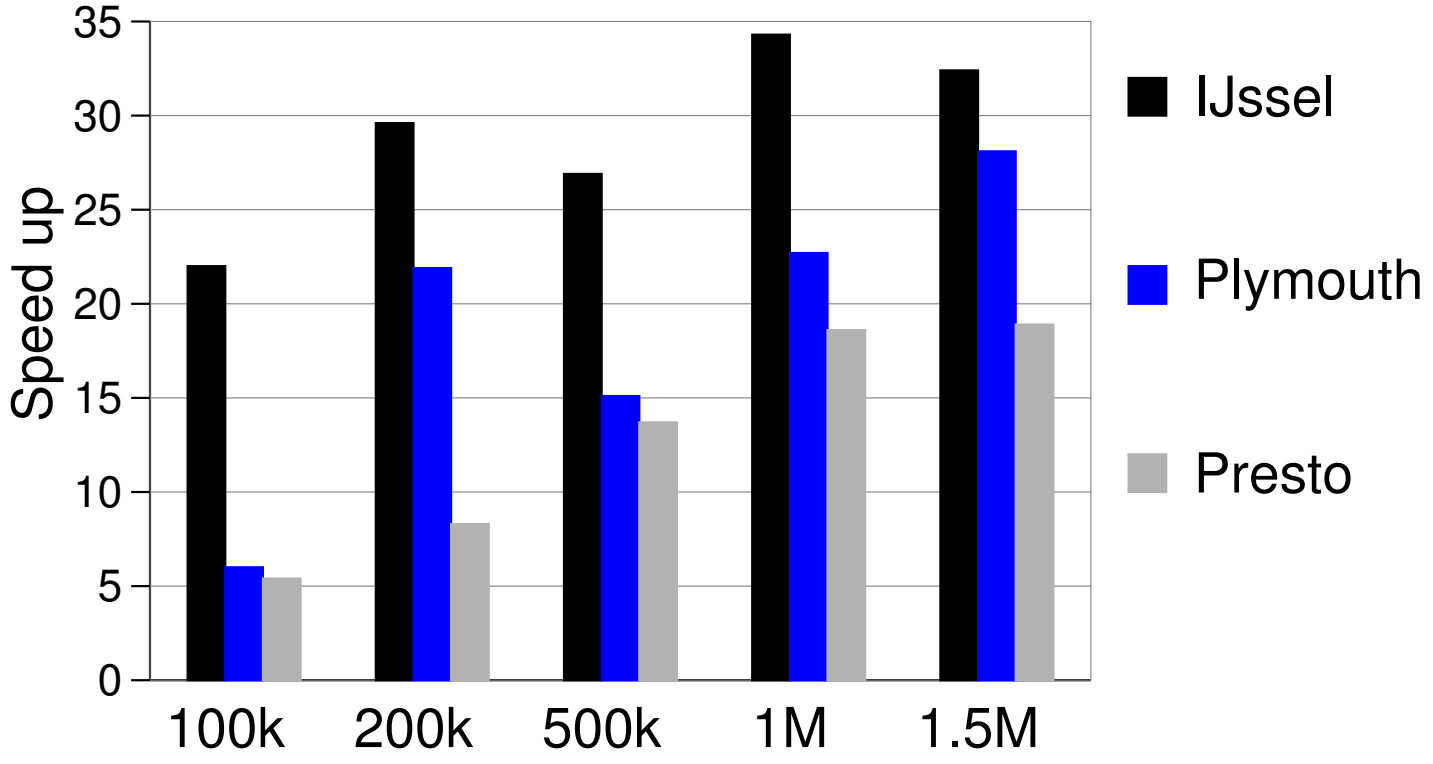
[b] An efficient preconditioned CG method for the solution of a class of layered problems with extreme contrasts in the coefficients. C. Vuik, A. Segal, J.A. Meijerink J. Comput. Phys. 1999.

3. Numerical results: ship simulator



- Including: 2D Poisson, Gelderse IJssel (NL), Plymouth Sound (UK)
- Realistic domains up to 1.5 million nodes

Numerical results: ship simulator



Speed up numbers for the realistic test problems.

Numerical results: Bubbly flow

$$Speedup = \frac{T_{CPU}}{T_{GPU}} \tag{8}$$

- Number of Unknowns = 128^3.
- Tolerance set to 10^{-6}.
- Density Contrast is 10^{-3}

Naming deflation vectors

- SD-i -> Sub-domain deflation with i vectors.
- LS-i -> Level-Set deflation with i vectors.
- LSSD-i -> Level-Set Sub-domain deflation with i vectors.

Numerical results: Bubbly flow

9 bubbles - 64 Sub-domains

	CPU	GPU-CUSP	
	DICCG(0)	DPCG(TNS)	
	SD-64	SD-63	LSSD-135
Number of Iterations	472	603	136
Total Time	81.39	13.61	5.58
Iteration Time	81.1	10.61	2.48
Speedup	-	7.64	32.7

Numerical results: Bubbly flow

9 bubbles - 512 Sub-domains

	CPU	GPU-CUSP	
	DICCG(0)	DPCG(TNS)	
	SD-512	SD-511	LSSD-583
Number of Iterations	67	81	81
Total Time	12.51	4.56	4.62
Iteration Time	12.18	1.56	1.62
Speedup	-	7.81	7.52

Paralution[a] results: Bubbly flow

Intel Xeon dual quad-core CPU versus NVIDIA K20 GPU

	ME-ILU-J	ILU(0)	FSAI	MCSGS	TNS
Iterations	210	142	163	203	175
CPU Time	9.324	17.1	19.53	9.843	**8.61**
GPU Time	2.74	5.165	6.68	2.841	**2.25**

Comparing **Deflated** PCG for different preconditioners

Grid Size - 128^3. 8 bubbles.

[a] http://www.paralution.com/

4. Conclusions

- ILU type preconditioners can be used on GPU's by a Neumann series approach or a carefull reordering
- Deflation type preconditioners are very suitable for GPU's
- The combination of Neumann series and Deflation preconditioners leads to robust and fast solvers on the GPU
- A special ordering of a red black reordering can lead to speedup of a factor 30-40 on the GPU.

Main question

Can ILU preconditioners be combined with GPU's?

Main question

Can ILU preconditioners be combined with GPU's?

YES

References

- H. Knibbe and C.W. Oosterlee and C. Vuik GPU implementation of a Helmholtz Krylov solver preconditioned by a shifted Laplace multigrid method Journal of Computational and Applied Mathematics, 236, pp. 281-293, 2011
- R. Gupta, M.B. van Gijzen and C. Vuik 3D Bubbly Flow Simulation on the GPU - Iterative Solution of a Linear System Using Sub-domain and Level-Set Deflation, 21st Euromicro International Conference on Parallel, Distributed and Network-Based Processing (PDP), 2013, ISBN 978-1-4673-5321-2, pp. 359-366, 2013
  http://ieeexplore.ieee.org/xpl/articleDetails.jsp?arnumber=6498576
- M. de Jong Developing a CUDA solver for large sparse matrices for MARIN, MSc Thesis, Delft University of Technology, 2012
  http://ta.twi.tudelft.nl/nw/users/vuik/numanal/jong_afst.pdf

- Rohit Gupta thesis defence is in the second half of 2014

For CV etc.: http://ta.twi.tudelft.nl/nw/users/rohit/