HSS Algorithms & Applications

Shivkumar Chandrasekaran
Bill Lyons   Tim Pals
University of California, Santa Barbara

Ming Gu
University of California, Berkeley

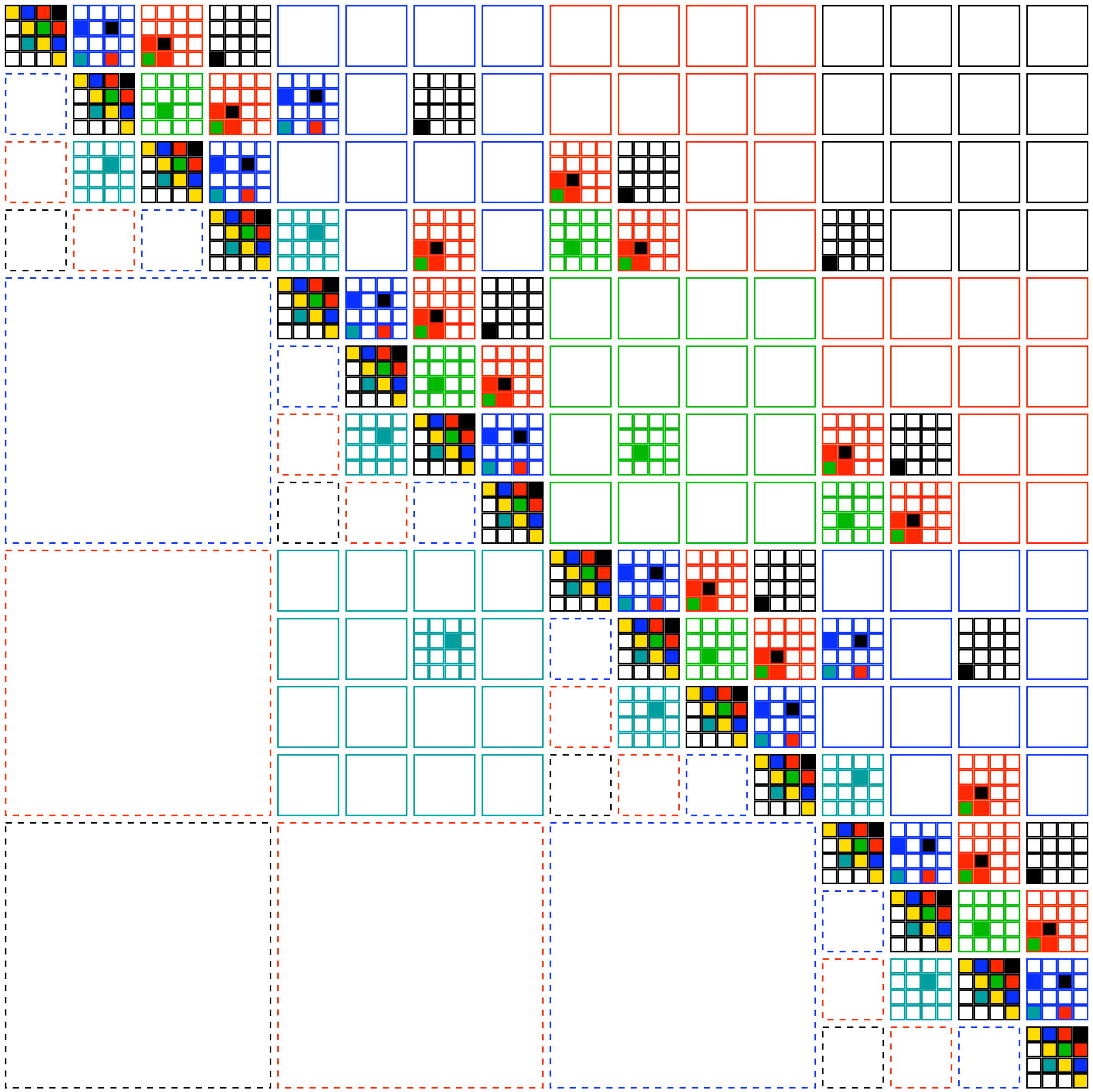
Dense Matrices

Key bottle-neck in computations

- Pseudo-spectral methods
- Fill-in for finite-element methods
- Boundary-element methods

Low Rank Structure

The blank squares have low-rank. The filled-in squares have full-rank. The color determines the recursive partitioning strategy.



$$A = \|z_i - z_j\|^{\alpha},\ z_i \in \mathcal{R}^2$$

Fast Matrix Algebra

- Rokhlin: Fast Multi-pole Method (FMM)
- Hackbusch: Hierarchical Matrices, H2
- Dewilde: Linear Systems Theory

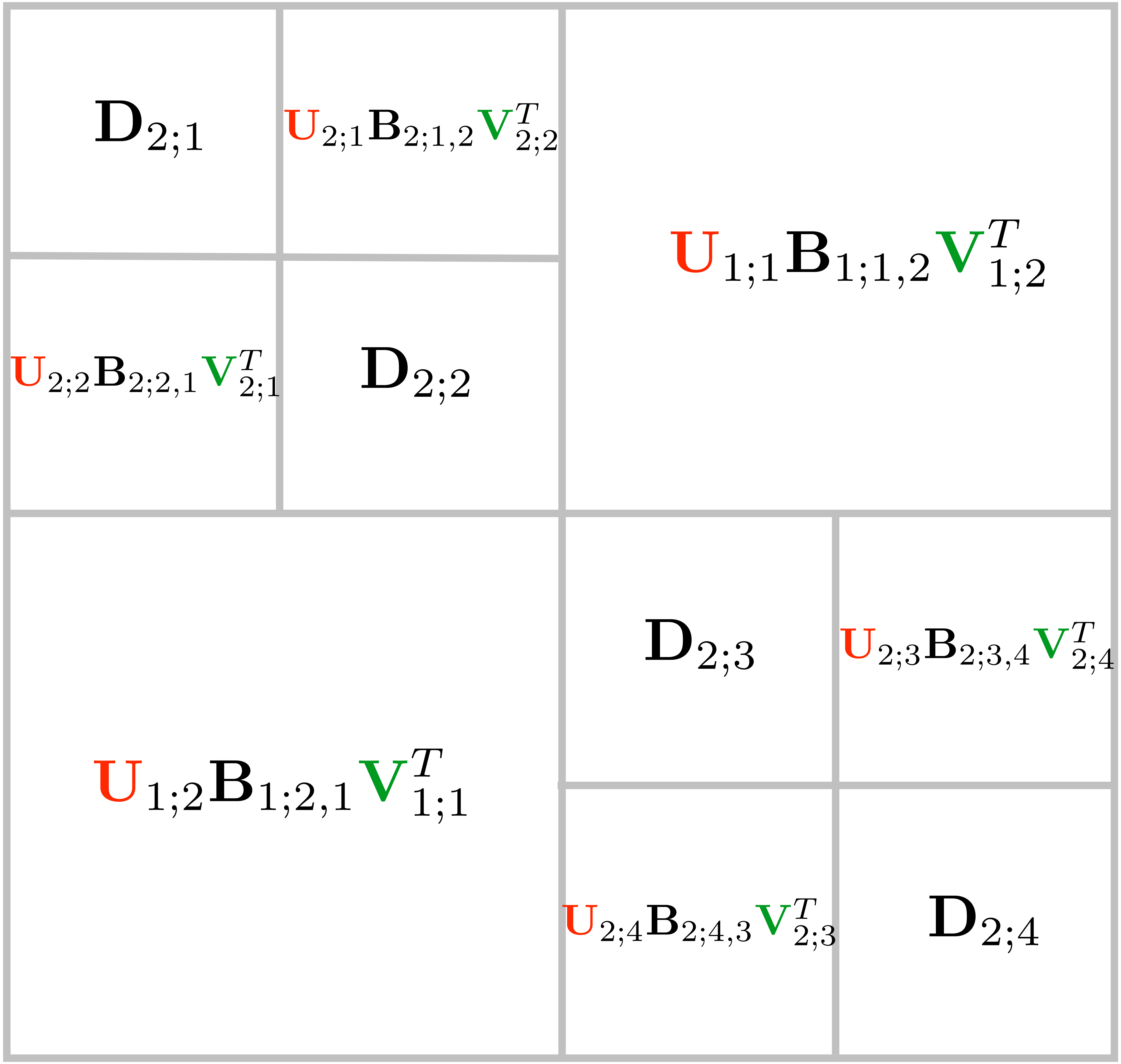
HSS

- Hierarchically Semi-Separable Representation
- Simplest FMM structure
- Exact, linear, stable solvers

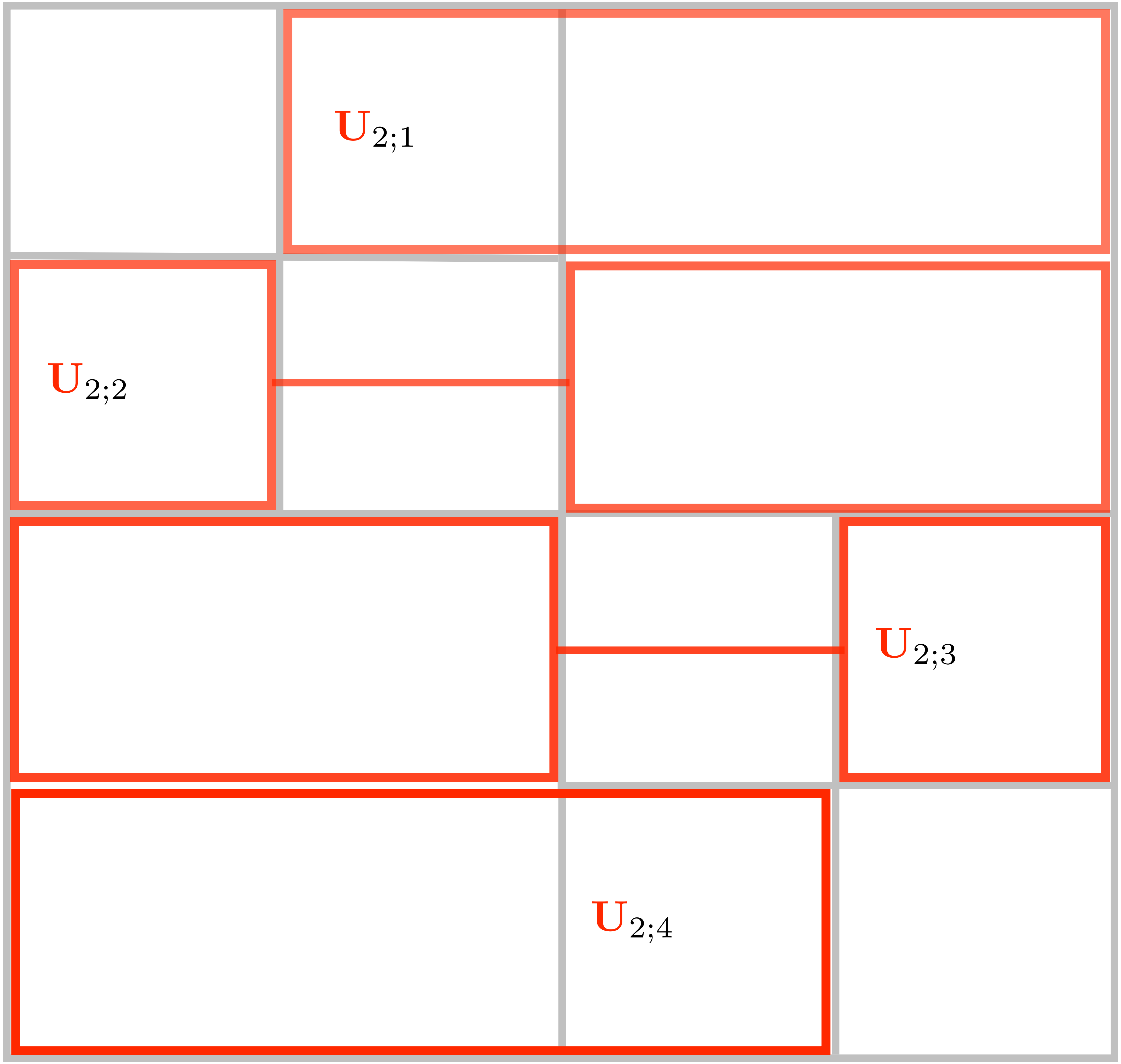
One level

$\mathbf{D}_{1;1}$	$\mathbf{U}_{1;1}\mathbf{B}_{1;1,2}\mathbf{V}_{1;2}^T$
$\mathbf{U}_{1;2}\mathbf{B}_{1;2,1}\mathbf{V}_{1;1}^T$	$\mathbf{D}_{1;2}$

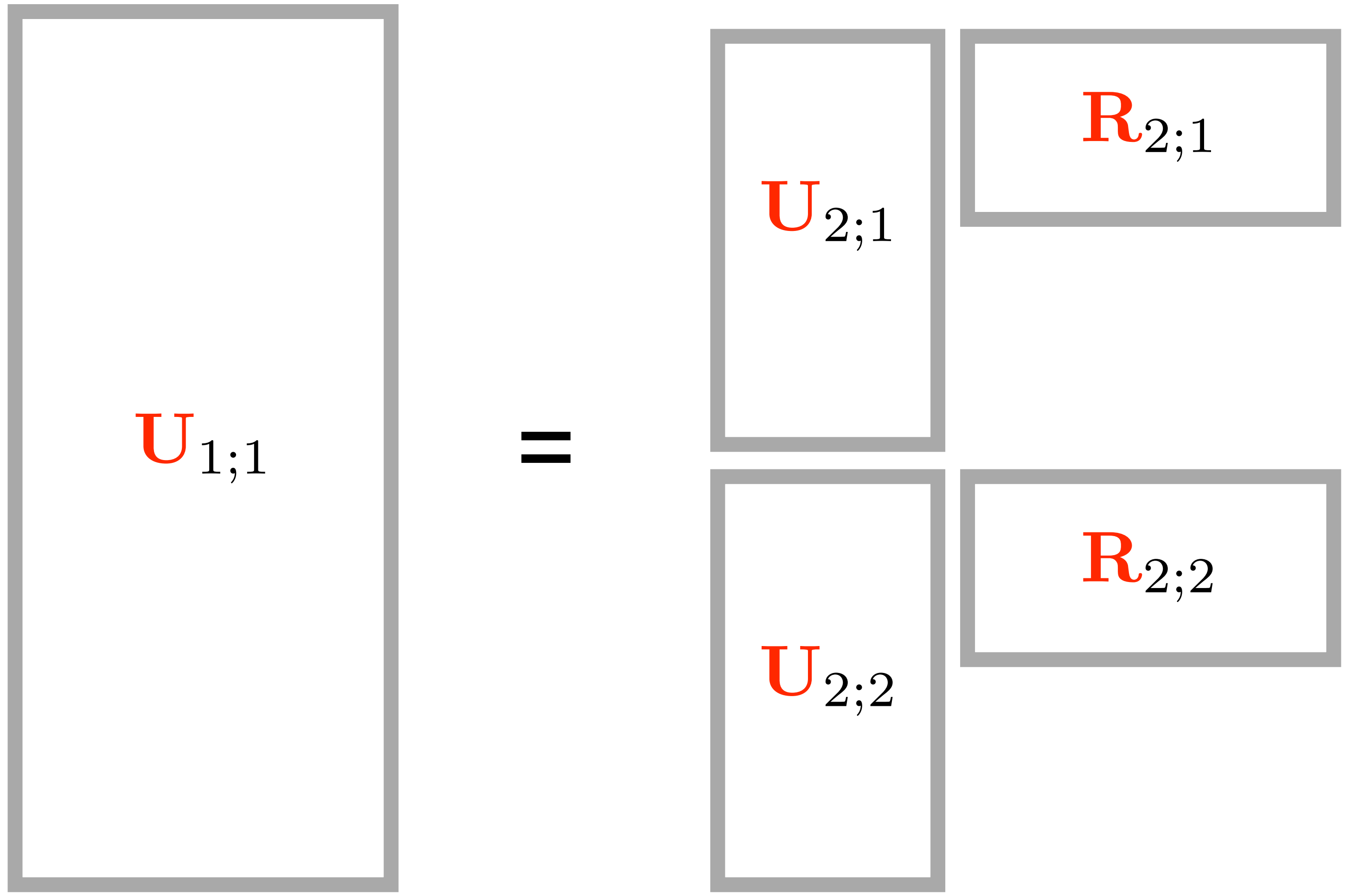
Two level


$\mathbf{D}_{2;1}$
$\mathbf{U}_{2;1}\mathbf{B}_{2;1,2}\mathbf{V}_{2;2}^T$
$\mathbf{U}_{1;1}\mathbf{B}_{1;1,2}\mathbf{V}_{1;2}^T$
$\mathbf{U}_{2;2}\mathbf{B}_{2;2,1}\mathbf{V}_{2;1}^T$
$\mathbf{D}_{2;2}$
$\mathbf{D}_{2;3}$
$\mathbf{U}_{2;3}\mathbf{B}_{2;3,4}\mathbf{V}_{2;4}^T$
$\mathbf{U}_{1;2}\mathbf{B}_{1;2,1}\mathbf{V}_{1;1}^T$
$\mathbf{U}_{2;4}\mathbf{B}_{2;4,3}\mathbf{V}_{2;3}^T$
$\mathbf{D}_{2;4}$

Column bases



Column Translation Operators

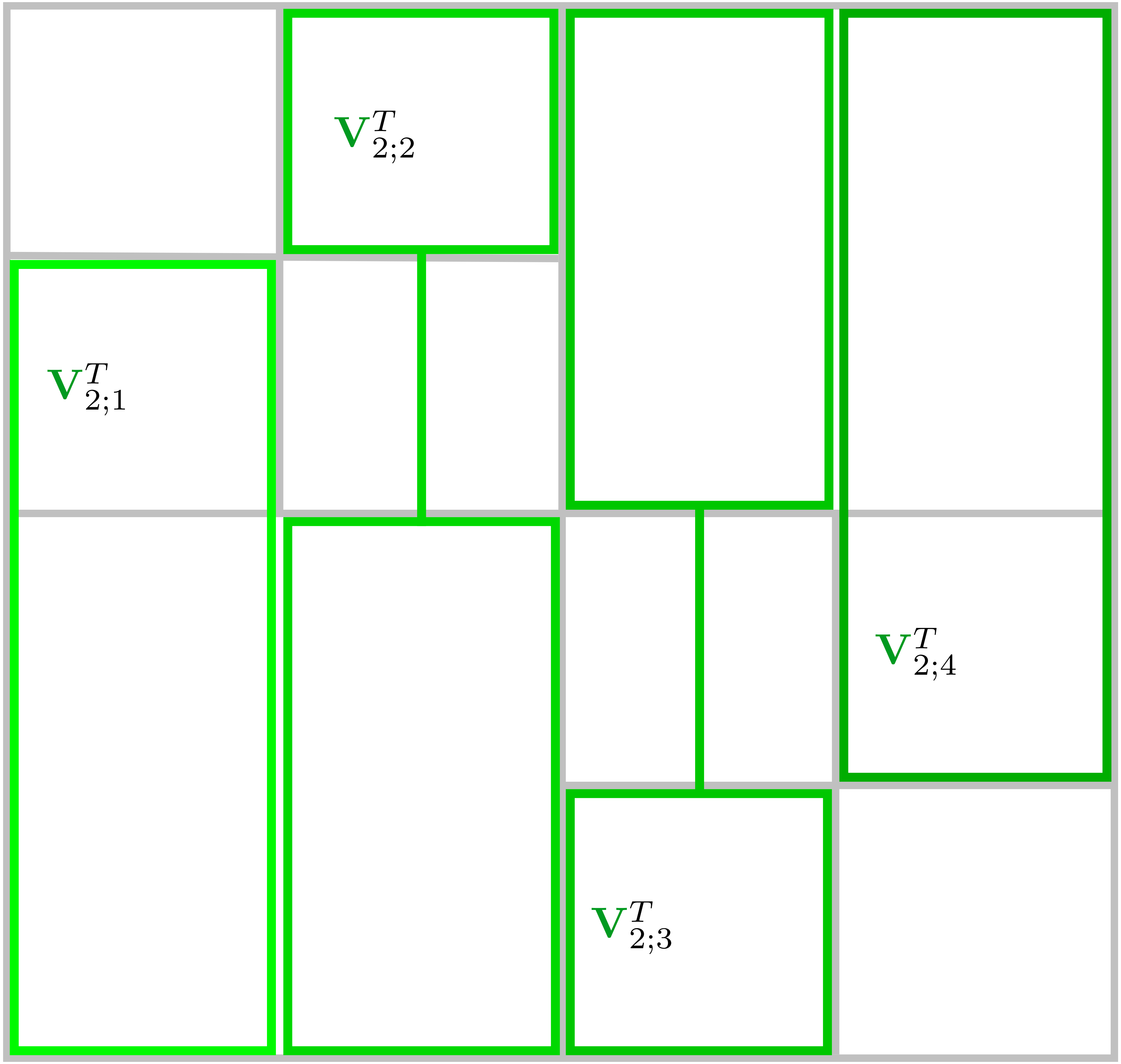


Similarly

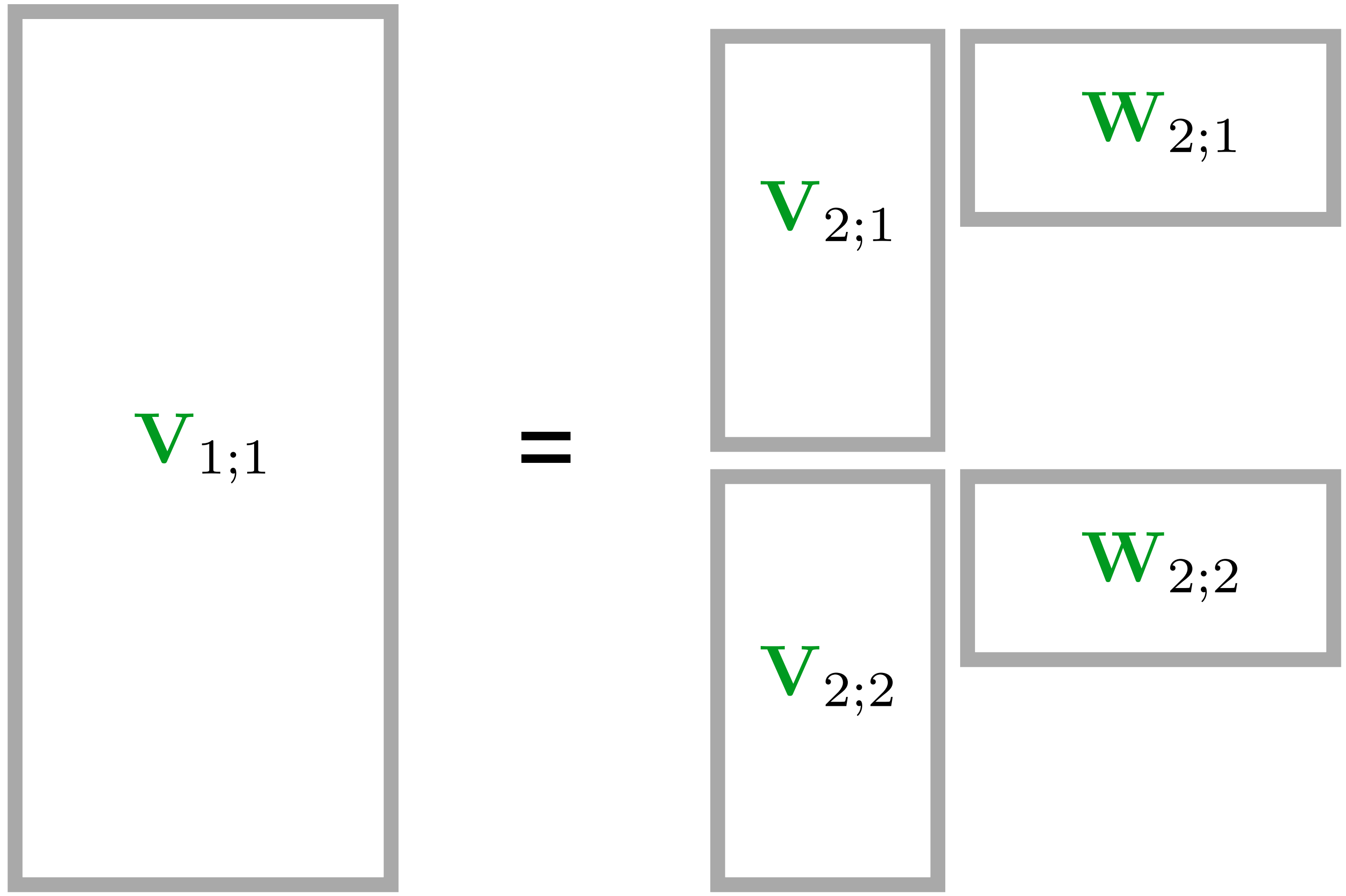
$$\mathbf{U}_{1;2} = \begin{pmatrix} \mathbf{U}_{2;3}\mathbf{R}_{2;3} \\ \mathbf{U}_{2;4}\mathbf{R}_{2;4} \end{pmatrix}$$

- $\mathbf{U}_{1;*}$ not needed and not stored
- $\mathbf{R}_{2;*}$ are smaller and stored

Row bases



Row Translation Operators

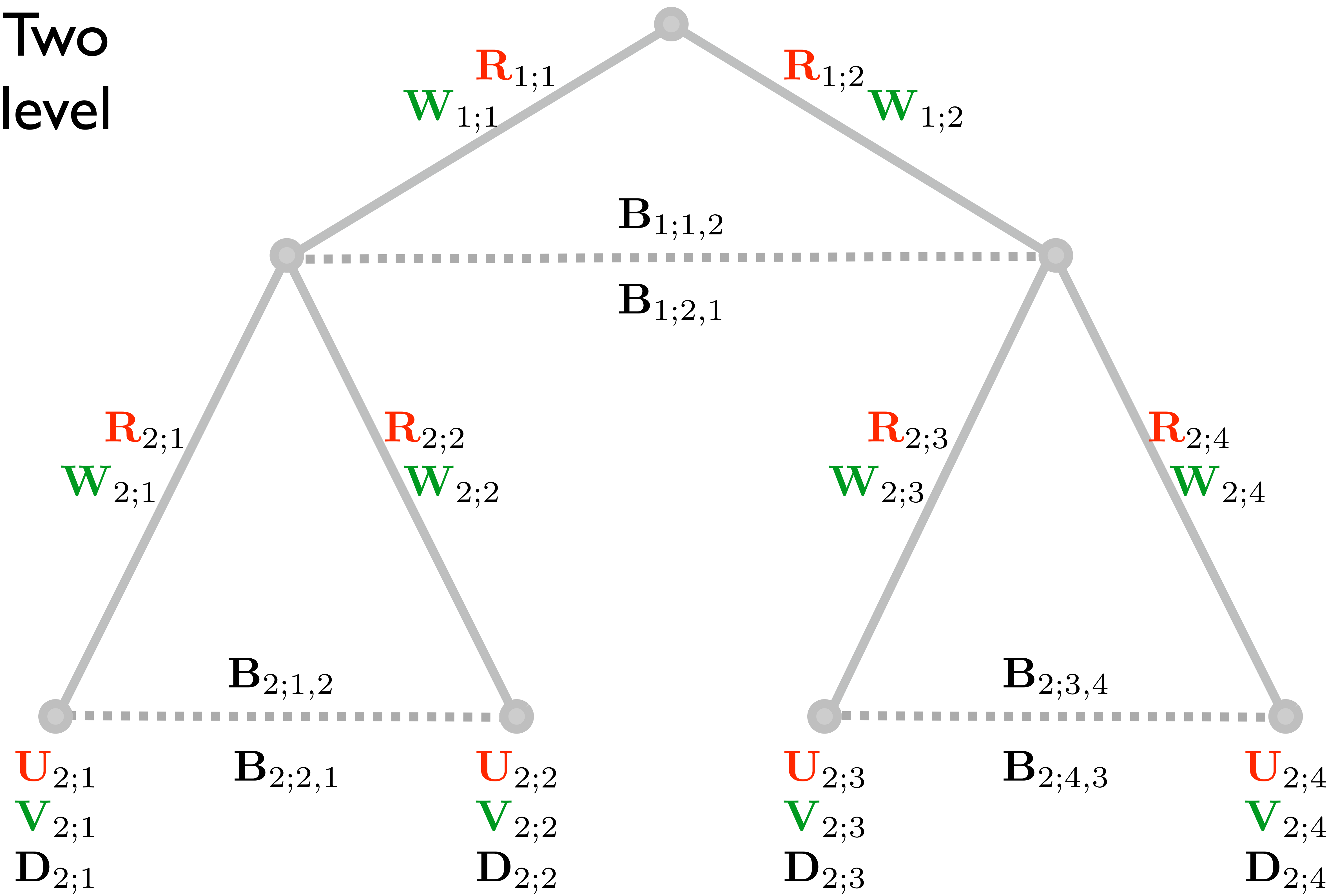


Similarly

$$\mathbf{V}_{1;2} = \begin{pmatrix} \mathbf{V}_{2;3}\mathbf{W}_{2;3} \\ \mathbf{V}_{2;4}\mathbf{W}_{2;4} \end{pmatrix}$$

- $\mathbf{V}_{1;*}$ not needed and not stored
- $\mathbf{W}_{2;*}$ are smaller and stored

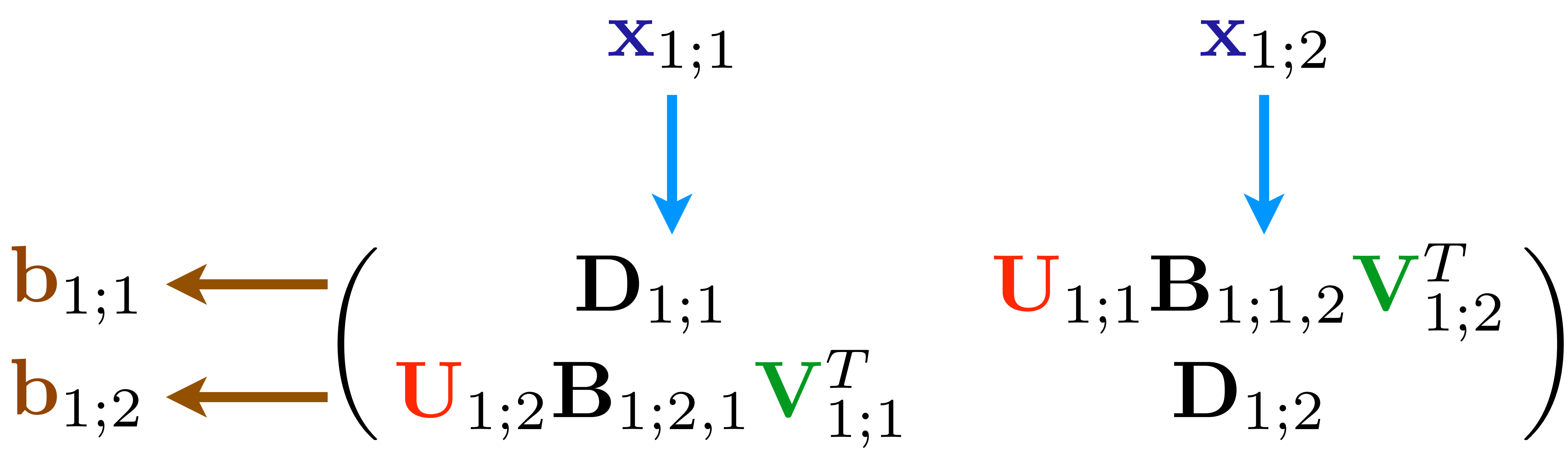
Two level



Binary Tree Representation

FMM (One Level)

$$\begin{pmatrix} \mathbf{b}_{1;1} \\ \mathbf{b}_{1;2} \end{pmatrix} = \begin{pmatrix} \mathbf{D}_{1;1} & \mathbf{U}_{1;1}\mathbf{B}_{1;1,2}\mathbf{V}_{1;2}^{T} \\ \mathbf{U}_{1;2}\mathbf{B}_{1;2,1}\mathbf{V}_{1;1}^{T} & \mathbf{D}_{1;2} \end{pmatrix} \begin{pmatrix} \mathbf{x}_{1;1} \\ \mathbf{x}_{1;2} \end{pmatrix}$$



FMM (One Level)...

$$\mathbf{g}_{1;i} = \mathbf{V}_{1;i}^{T}\mathbf{x}_{1;i}$$

$$\mathbf{f}_{1;i} = \mathbf{B}_{1;i,j}\mathbf{g}_{1;i}$$

$$\mathbf{b}_{1;i} = \mathbf{U}_{1;i}\mathbf{f}_{1;i} + \mathbf{D}_{1;i}\mathbf{x}_{1;i}$$

FMM (Two Level)

$$\mathbf{x}_{2;1} \quad \mathbf{x}_{2;2} \quad \mathbf{x}_{2;3} \quad \mathbf{x}_{2;4}$$

$$\begin{matrix} \mathbf{b}_{2;1} \\ \mathbf{b}_{2;2} \\ \mathbf{b}_{2;3} \\ \mathbf{b}_{2;4} \end{matrix} \leftarrow \left(\begin{array}{c|c} \begin{matrix} \mathbf{D}_{2;1} & \mathbf{U}_{2;1}\mathbf{B}_{2;1,2}\mathbf{V}^T_{2;2} \\ \mathbf{U}_{2;2}\mathbf{B}_{2;2,1}\mathbf{V}^T_{2;1} & \mathbf{D}_{2;2} \end{matrix} & \mathbf{U}_{1;1}\mathbf{B}_{1;1,2}\mathbf{V}^T_{1;2} \\ \hline \mathbf{U}_{1;2}\mathbf{B}_{1;2,1}\mathbf{V}^T_{1;1} & \begin{matrix} \mathbf{D}_{2;3} & \mathbf{U}_{2;3}\mathbf{B}_{2;3,4}\mathbf{V}^T_{2;4} \\ \mathbf{U}_{2;4}\mathbf{B}_{2;4,3}\mathbf{V}^T_{2;3} & \mathbf{D}_{2;4} \end{matrix} \end{array}\right)$$

FMM (Two Level)...

$$\mathbf{g}_{k;i} = \mathbf{V}_{k;i}^T \mathbf{x}_{k;i}$$

But $\mathbf{V}_{1;i}$ is not available

$$\begin{aligned}
\mathbf{g}_{1;1} &= \mathbf{V}_{1;1}^T \mathbf{x}_{1;1} \\
&= \begin{pmatrix} \mathbf{W}_{2;1}^T \mathbf{V}_{2;1}^T & \mathbf{W}_{2;2}^T \mathbf{V}_{2;2}^T \end{pmatrix} \begin{pmatrix} \mathbf{x}_{2;1} \\ \mathbf{x}_{2;2} \end{pmatrix} \\
&= \mathbf{W}_{2;1}^T \mathbf{g}_{2;1} + \mathbf{W}_{2;2}^T \mathbf{g}_{2;2}
\end{aligned}$$

FMM (Two Level)...

- At output try the formula

$$\mathbf{b}_{k;i} = \mathbf{U}_{k;i}\mathbf{f}_{k;i} + \mathbf{D}_{k;i}\mathbf{x}_{k;i}$$

- Obviously

$$\mathbf{f}_{1;i} = \mathbf{B}_{1;i,j}\mathbf{g}_{1;i}$$

- But $\mathbf{U}_{1;i}$ is not available

FMM (Two Level)...

Let us look at first output line

$$\mathbf{b}_{2;1} = \mathbf{D}_{2;1}\mathbf{x}_{2;1} + \mathbf{U}_{2;1}\mathbf{B}_{2;1,2}\mathbf{g}_{2;2} + \mathbf{U}_{2;1}\mathbf{R}_{2;1}\mathbf{B}_{1;1,2}\mathbf{g}_{1;2}$$

$$= \mathbf{D}_{2;1}\mathbf{x}_{2;1} + \mathbf{U}_{2;1}\underbrace{(\mathbf{B}_{2;1,2}\mathbf{g}_{2;2} + \mathbf{R}_{2;1}\underbrace{\mathbf{B}_{1;1,2}\mathbf{g}_{1;2}}_{\mathbf{f}_{1;1}})}_{\mathbf{f}_{2;1}}$$

Hence

$$\mathbf{f}_{2;1} = \mathbf{B}_{2;1,2}\mathbf{g}_{2;2} + \mathbf{R}_{2;1}\mathbf{f}_{1;1}$$

FMM

Up-sweep recursions

$$\mathbf{g}_{k;i} = \mathbf{V}_{k;i}^T \mathbf{x}_{k;i}$$

$$\mathbf{g}_{k-1;i} = \mathbf{W}_{k;2i-1}^T \mathbf{g}_{k;2i-1} + \mathbf{W}_{k;2i}^T \mathbf{g}_{k;2i}$$

Down-sweep recursions

$$\mathbf{f}_{0;1} = (\,\cdot\,)$$

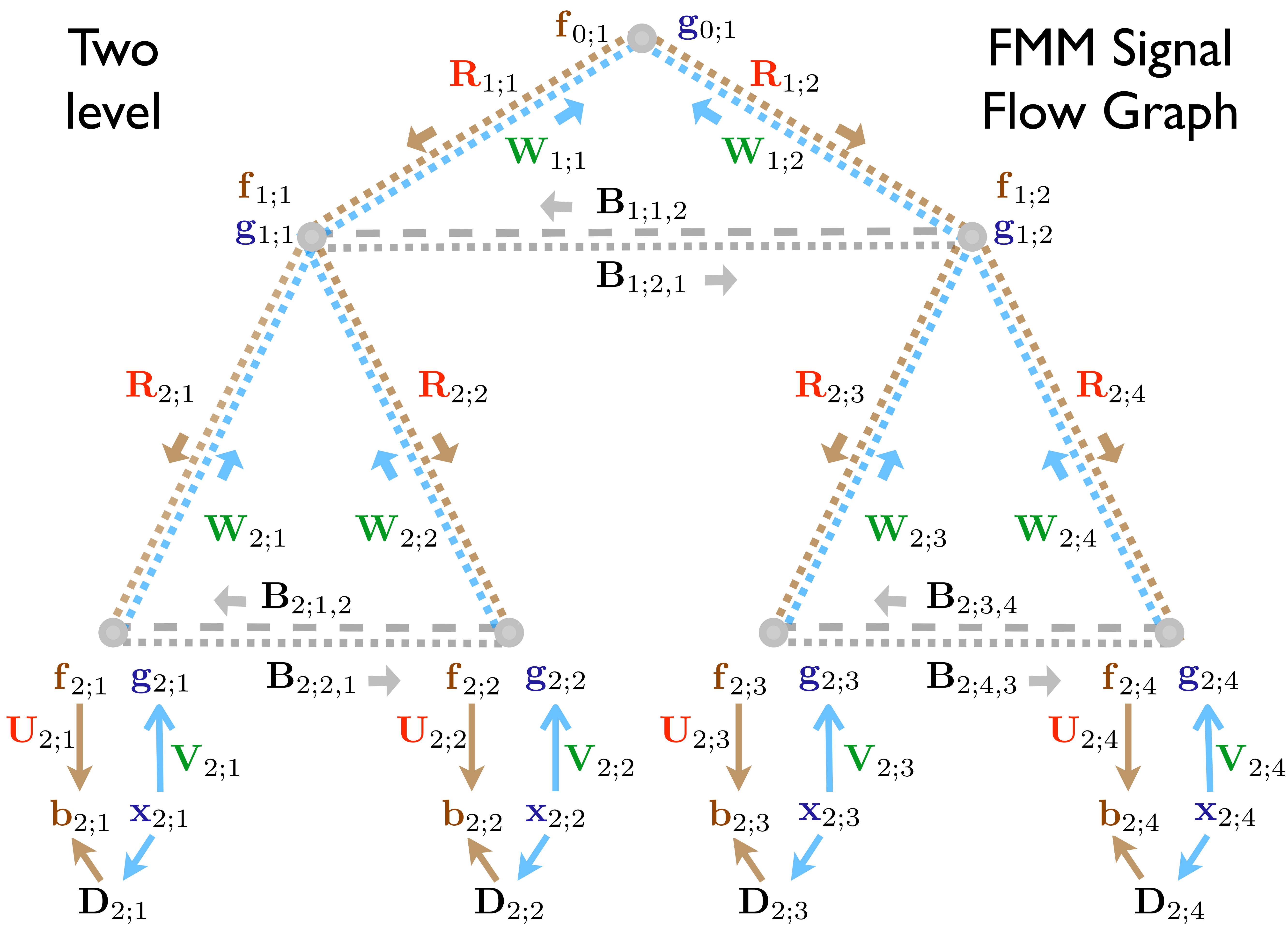
$$\mathbf{f}_{k;2i-1} = \mathbf{B}_{k;2i-1,2i} \mathbf{g}_{k;2i} + \mathbf{R}_{k;2i-1} \mathbf{f}_{k-1;i}$$

$$\mathbf{f}_{k;2i} = \mathbf{B}_{k;2i,2i-1} \mathbf{g}_{k;2i-1} + \mathbf{R}_{k;2i} \mathbf{f}_{k-1;i}$$

Outputs

$$\mathbf{b}_{k;i} = \mathbf{U}_{k;i} \mathbf{f}_{k;i} + \mathbf{D}_{k;i} \mathbf{x}_{k;i}$$

Two level FMM Signal Flow Graph



Sparse Representation

$$\begin{pmatrix} \mathbf{D} & 0 & \mathbf{U}\mathbf{P}_{\text{leaf}} \\ 0 & \mathbf{B}\mathbf{Z}_{\leftrightarrow} & \mathbf{R}\mathbf{Z}_{\downarrow} - I \\ \mathbf{P}_{\text{leaf}}^{H}\mathbf{V}^{H} & \mathbf{Z}_{\downarrow}^{H}\mathbf{W}^{H} - I & 0 \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{g} \\ \mathbf{f} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ 0 \\ 0 \end{pmatrix}$$

$\mathbf{D}, \mathbf{B}, \mathbf{U}, \mathbf{R}, \mathbf{V}, \mathbf{W}$ are diagonal matrices

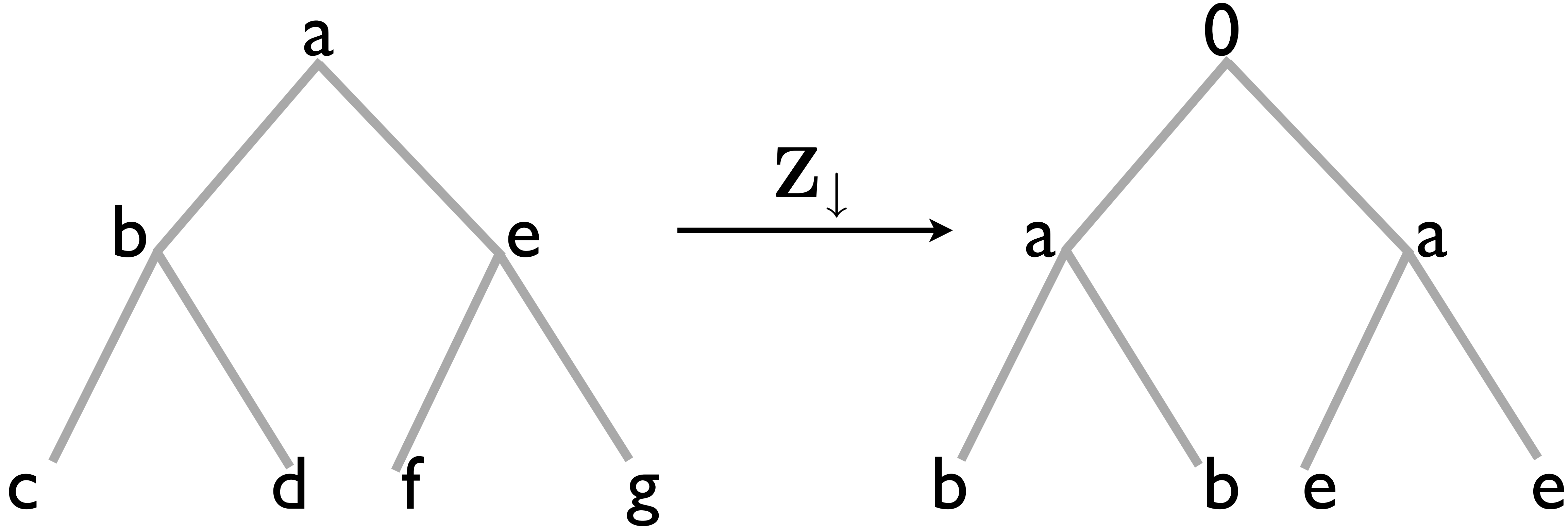
$\mathbf{Z}_{\downarrow}$ is a shift down matrix acting on trees

$\mathbf{Z}_{\leftrightarrow}$ exchanges siblings on the tree

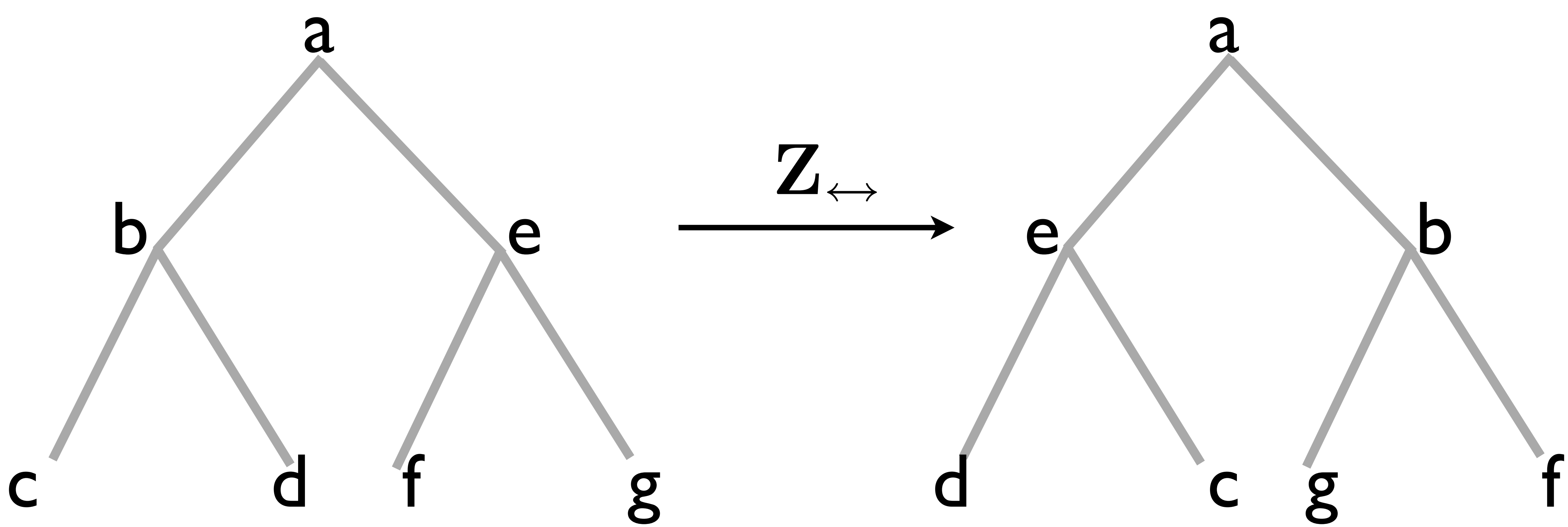
$\mathbf{P}_{\text{leaf}}$ projects onto leaf indices

Fast Solvers

- The binary tree has good separators
- Hence we have fast (*LU* and *QR*) solvers



$$\underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 & 0 \\ I & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 & 0 \end{pmatrix}}_{\mathbf{z}_{\downarrow}} \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{pmatrix} = \begin{pmatrix} 0 \\ a \\ b \\ b \\ a \\ e \\ e \end{pmatrix}$$



$$\underbrace{\begin{pmatrix} I & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I \\ 0 & 0 & 0 & 0 & 0 & I & 0 \end{pmatrix}}_{\mathbf{Z}_{\leftrightarrow}} \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \\ g \end{pmatrix} = \begin{pmatrix} a \\ e \\ d \\ c \\ b \\ g \\ f \end{pmatrix}$$

Diffusion Equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad -1 \leq x \leq 1$$

$$u(x,0) = \exp x^2$$

$$u(\pm 1, t) = \sqrt{\frac{1}{t+1}} \exp\left(-\frac{1}{4(t+1)}\right), \quad t > 0$$

Fast Pseudo-spectral Solver

- Pseudo-spectral differentiation matrix has compact HSS representation
- Non-periodic boundary conditions are a snap
- Given basic HSS forms system can be assembled in linear time
- Overall complexity is linear

100 Crank-Nicholson time steps

Gauss-Lobatto points	CPU time (seconds)	Error (1E-6)
200	2.13	1.20
400	5.23	1.19
800	14.1	1.19
1600	38.5	1.20
3200	87.4	1.22
6400	213	1.44

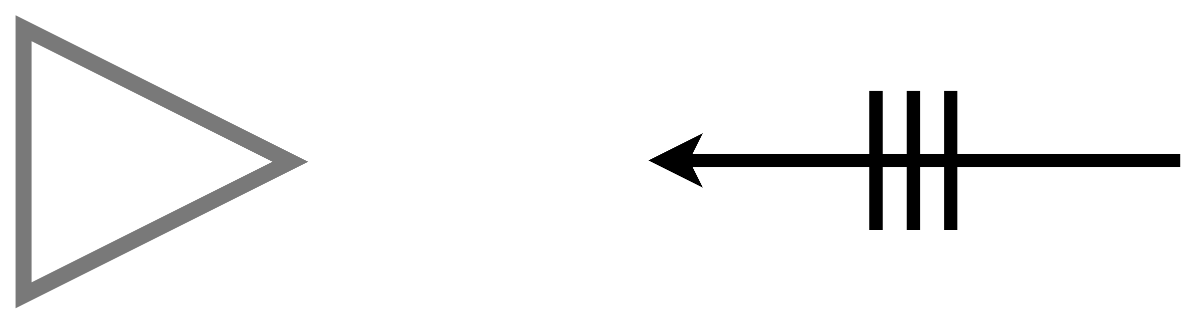
Fast Solver Timings (seconds)

$$A_{i,j} = \begin{cases} \frac{\sin(\pi\|x_i - x_j\|)}{\|x_i - x_j\|}, & i \neq j, \\ 1, & i = j \end{cases}$$

Random points on the sphere in nested dissection order

Number of points	1E-4	1E-8
100	0.01	0.01
200	0.03	0.07
400	0.07	0.21
800	0.13	0.42
1600	0.26	0.90
3200	0.50	1.48
6400	0.89	2.57
12800	1.58	4.05
25600	2.71	6.35
51200	5.11	11.48

Fast Inversion of FMM



- Classical exterior scattering (Helmholtz equation)
- Wavenumber = 100
- Boundary integral equation formulation
- FMM relative accuracy of 1E-10

Fast FMM Inversion

Timing in seconds

Number of points	Dense *LU*	GMRES-FMM	Sparse *LU*
1536	12.36	13.40	2.62
2304	36.24	20.03	2.73
3072	88.69	42.13	3.79
3840	(173)	53.13	4.61
4608	(299)	68.56	4.94
5376	(475)	96.65	5.54

AB = C

Define g and f via

$$\mathbf{g}_{k;i} = \mathbf{V}_{k;i}^{H}(A)\mathbf{U}_{k;i}(B)$$

$$\mathbf{D}_{k;i}(C) = \mathbf{D}_{k;i}(A)\mathbf{D}_{k;i}(B) + \mathbf{U}_{k;i}(A)\mathbf{f}_{k;i}\mathbf{V}_{k;i}^{H}(B)$$

Up-sweep and down-sweep recursions

$$\mathbf{g}_{k-1;i} = \mathbf{W}_{k;2i-1}^{H}(A)\mathbf{g}_{k;2i-1}\mathbf{R}_{k;2i-1}(B) + \mathbf{W}_{k;2i}^{H}(A)\mathbf{g}_{k;2i}\mathbf{R}_{k;2i}(B)$$

$$\mathbf{f}_{k;i} = \mathbf{B}_{k;i,j}(A)\mathbf{g}_{k;j}\mathbf{B}_{k;j,i}(B) + \mathbf{R}_{k;i}(A)\mathbf{f}_{k-1;\lceil \frac{i}{2} \rceil}\mathbf{W}_{k;i}^{H}(B)$$

AB = C

$$\mathbf{U}_{k;i}(C) = \begin{pmatrix} \mathbf{U}_{k;i}(A) & \mathbf{D}_{k;i}(A)\mathbf{U}_{k;i}(B) \end{pmatrix}$$

$$\mathbf{V}_{k;i}(C) = \begin{pmatrix} \mathbf{D}^H_{k;i}(B)\mathbf{V}_{k;i}(A) & \mathbf{V}_{k;i}(B) \end{pmatrix}$$

$$\mathbf{R}_{k;i}(C) = \begin{pmatrix} \mathbf{R}_{k;i}(A) & \mathbf{B}_{k;i,j}(A)\mathbf{g}_{k;j}\mathbf{R}_{k;j}(B) \\ & \mathbf{R}_{k;i}(B) \end{pmatrix}$$

$$\mathbf{W}_{k;i}(C) = \begin{pmatrix} \mathbf{W}_{k;i}(A) & \\ \mathbf{B}^H_{k;j,i}(B)\mathbf{g}^H_{k;j}\mathbf{W}_{k;j}(A) & \mathbf{W}_{k;i}(B) \end{pmatrix}$$

$$\mathbf{B}_{k;i,j}(C) = \begin{pmatrix} \mathbf{B}_{k;i,j}(A) & \mathbf{R}_{k;i}(A)\mathbf{f}_{k-1;\lceil \frac{i}{2} \rceil}\mathbf{W}^H_{k;j}(B) \\ & \mathbf{B}_{k;i,j}(B) \end{pmatrix}$$