PARALLEL FAST GAUSS TRANSFORM

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PROBLEM STATEMENT

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Fast algorithms to compute discrete sums of the form:

$$F(x_j) = \sum_{k=1}^{N} G_\delta(\|x_j - y_k\|) f(y_k) \quad \text{at} \quad \{x_j \,|\, j = 1, \ldots, N\}$$

$x \rightarrow$ targets

$y \rightarrow$ sources

$f \rightarrow$ source strength

$x, y \in [0,1]^d$

G_δ is a *Gaussian-type* kernel

space-limited

band-limited

e.g., $G_\delta = \|x\|^2 e^{-\frac{\|x\|^2}{\delta}}$

Näive algorithm is $\mathcal{O}(N^2)$

MOTIVATION

PDE

$$\partial_t u = \triangle u \quad \text{in} \quad \omega$$
$$\partial u / \partial n = g \quad \text{on} \quad \gamma$$

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Potential Theory →

$$-\frac{1}{2}\mu + \mathcal{S}[\mu] = f$$
$$\mathcal{S}[\sigma] = \int_0^t \int_{\Gamma(y)} \frac{\sigma e^{-\frac{\|x-y\|^2}{4(t-\tau)}}}{(4\pi(t-\tau))^{d/2}} \, d\Gamma d\tau$$

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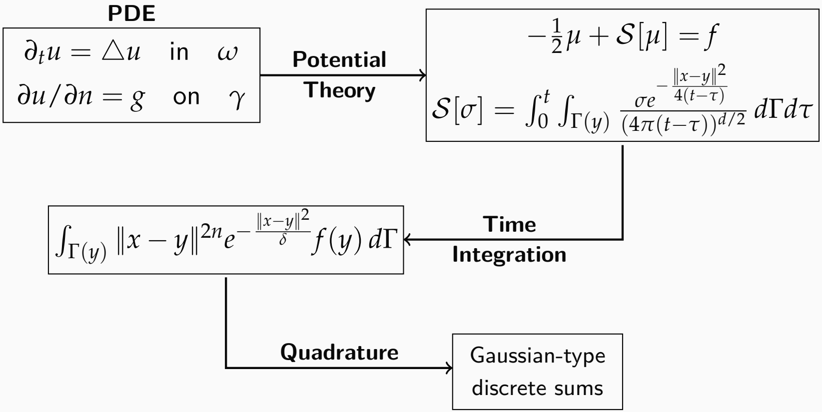
Time Integration →

$$\int_{\Gamma(y)} \|x-y\|^{2n} e^{-\frac{\|x-y\|^2}{\delta}} f(y) \, d\Gamma$$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$\partial_t u = \triangle u$ in ω
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Time Integration
$\int_{\Gamma(y)} \|x-y\|^{2n} e^{-\frac{\|x-y\|^2}{\delta}} f(y) \, d\Gamma$
Quadrature
Gaussian-type discrete sums

PDE		Kernels
Diffusion	$\partial_t u = \triangle u$	$\|x\|^{2n} e^{-\frac{\|x\|^2}{\delta}}$
Reaction-diffusion	$\partial_t u = \triangle u + u^2$	
Unsteady Stokes	$\partial_t \mathbf{u} = -\nabla P + \triangle \mathbf{u}$	$\left(\mathbf{I} - \frac{2x\otimes x}{\|x\|^2}\right) e^{-\frac{\|x\|^2}{\delta}}$
Navier-Stokes	$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla P + \triangle \mathbf{u}$	$\left(\mathbf{I} - \frac{4x\otimes x}{\|x\|^2}\right)\left(\frac{1-e^{-\frac{\|x\|^2}{\delta}}}{\|x\|^2}\right)$
		$\left(\mathbf{I} - \frac{4x\otimes x}{\|x\|^2}\right)\left(\delta\,\frac{1-e^{-\frac{\|x\|^2}{\delta}}}{\|x\|^2} - e^{-\frac{\|x\|^2}{\delta}}\right)$

RELATED WORK

Sequential

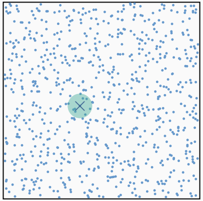
Greengard & Strain, 1991	FGT - Hermite expansions
Strain, 1991	variable scales
Greengard & Sun, 1998	Plane wave expansions
Sun & Bao, 2002	Kronecker-product rep.
Yang et al., 2003	high-dimensional FGT for KDEs
Spivak et al., 2010	Generalized FGT

Parallel

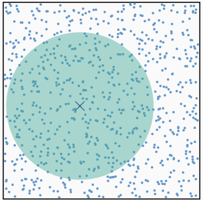
Yamamato, 2006	1D, $n_p \leq 16, N = \mathcal{O}(100)$
Yokota et al., 2009	RBFs, not optimal if Gaussian spread is large

Overview of FGT

$e^{-\frac{\|x-y\|^2}{\delta}}$



small δ



large δ

δ controls the decay of the kernel

If δ is small,

```
for each x
      F(x) = Σ_{y∈I[x]} G_δ(‖x − y‖) f(y)
end
```

$$F(x) = \sum_{y \in \mathcal{I}[x]} G_\delta(\|x - y\|) f(y)$$

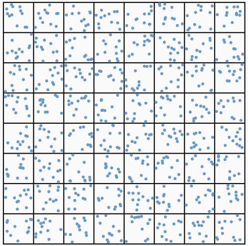
Sequential complexity: $\mathcal{O}(p^d N)$

Embarassingly parallel

EXPANSION

$$e^{-\|x-y\|^2/\delta} \approx \sum_{|k|\leq p} \hat{G}(k)\, e^{i\lambda k\cdot(x-y)}$$

$$\hat{G}(k) = \left(\frac{L}{2p\sqrt{\pi}}\right)^3 e^{-\frac{\lambda^2|k|^2\delta}{4}}, \quad \lambda = \frac{L}{p\sqrt{\delta}}$$



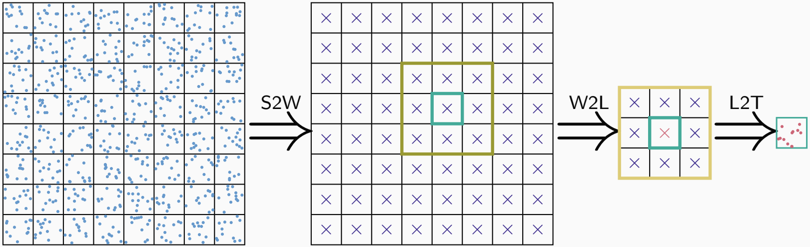
Partition the domain into uniform boxes of size $\sqrt{\delta}$

A fixed number (K^d) of neighboring boxes influence targets in a particular box

(**S2W**) Sources to Wave expansions $\mathcal{O}(p^d N)$
$$w_k = \sum_{y \in B} f(y) e^{i\lambda k \cdot (c^B - y)}$$

(**W2L**) Wave to Local expansions $\mathcal{O}(K^d p^d N_{\text{box}})$
$$v_k + = w_k e^{i\lambda k \cdot (c^D - c^B)}$$

(**L2T**) Local expansion to Targets $\mathcal{O}(p^d N)$
$$F(x) = \sum_{|k| \leq p} \hat{G}(k) v_k e^{i\lambda k \cdot (x - c^D)}$$

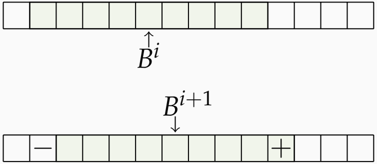


FGT: TRANSLATION

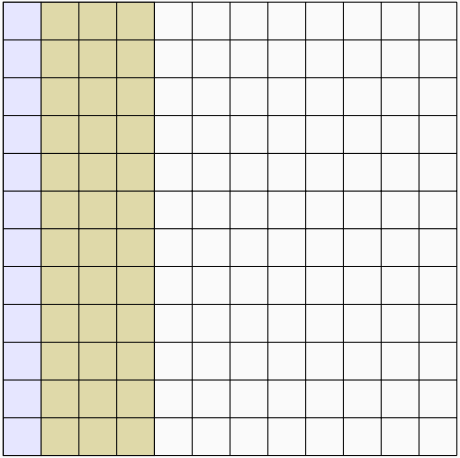
Reduces per box translation cost

$$K^3p^3 \to 9p^3$$

(K $=$ 13 for $\epsilon = 10^{-12}$)



$$v^{j+1} = \beta v^j - \alpha^l w^l + \alpha^r w^r$$



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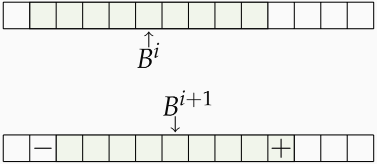

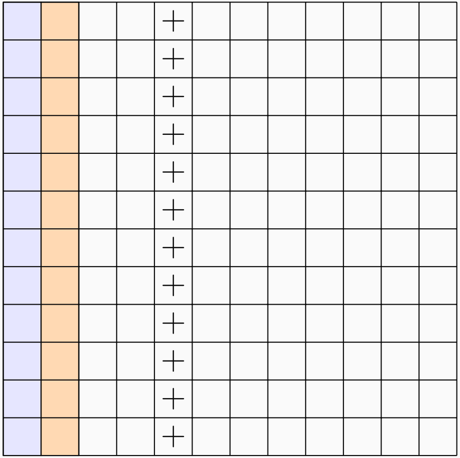

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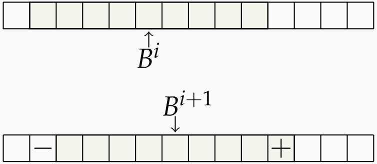

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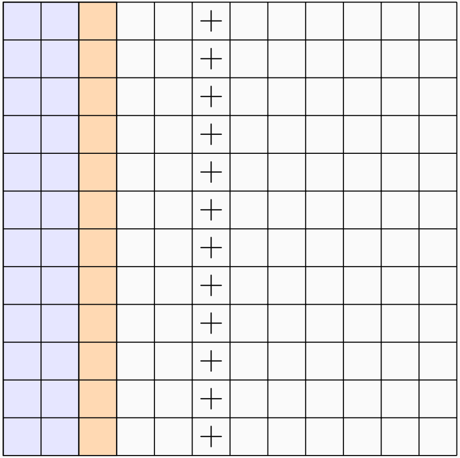

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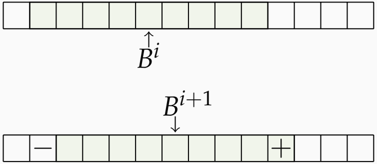

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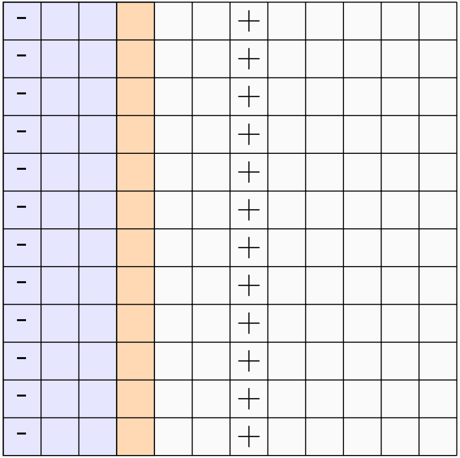

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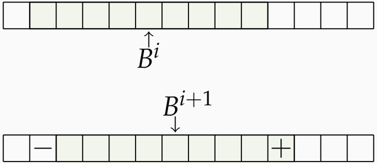

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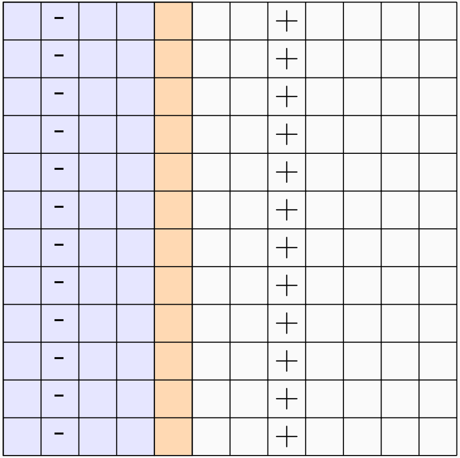

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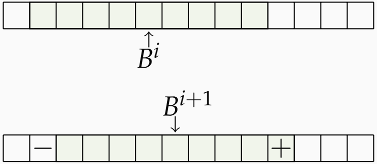

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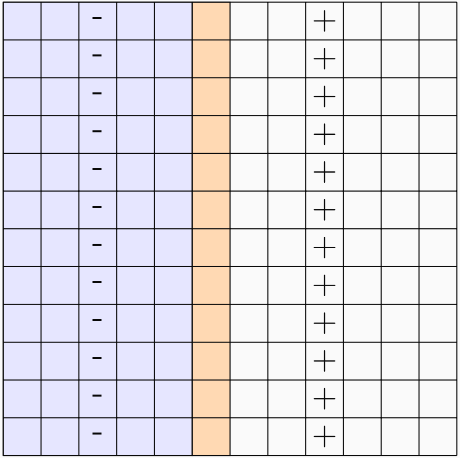

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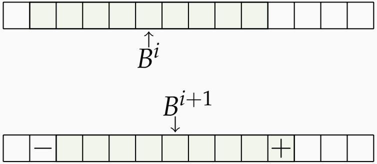

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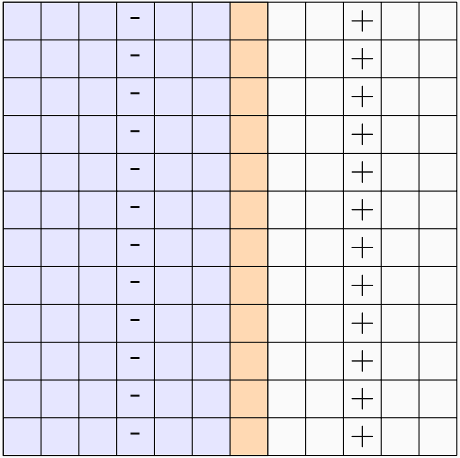

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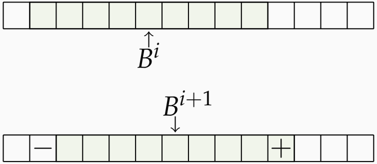

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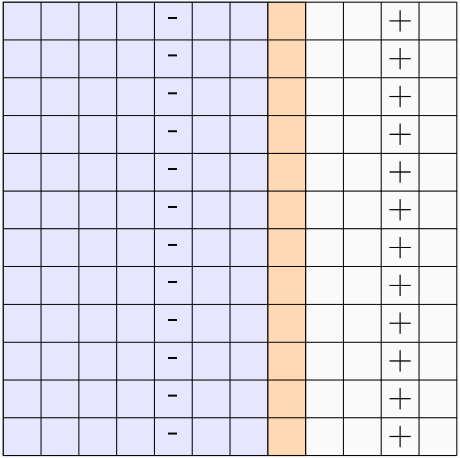

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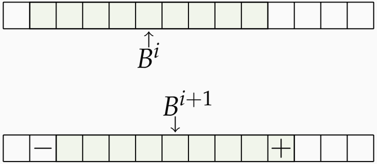

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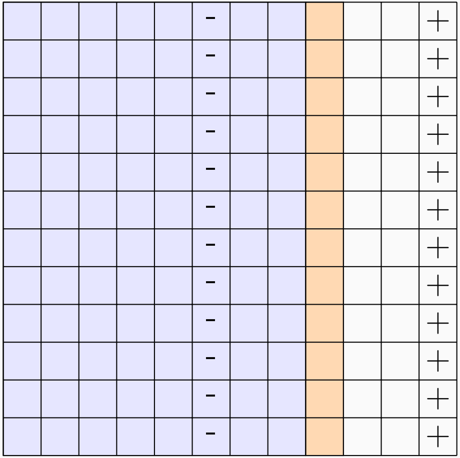

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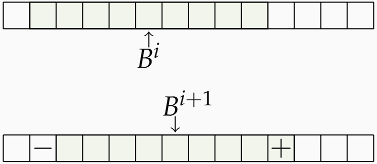

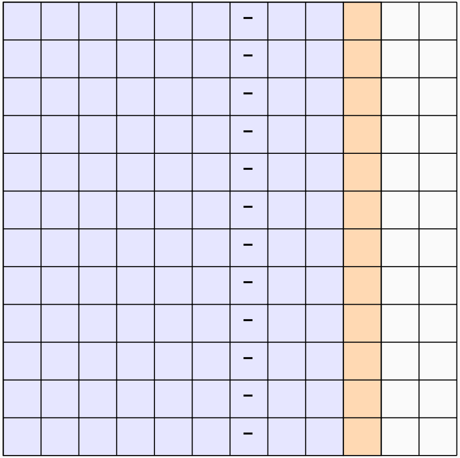

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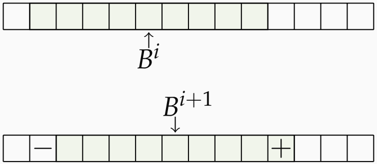

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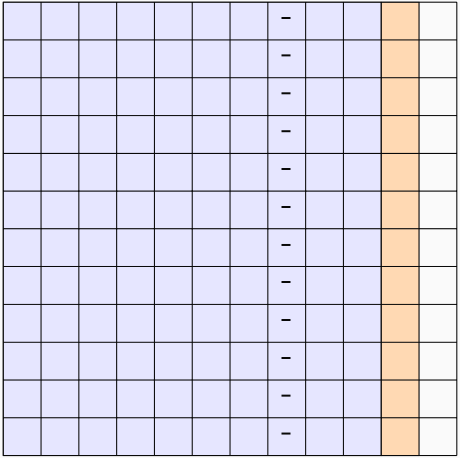

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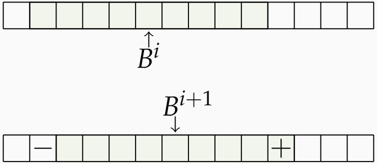

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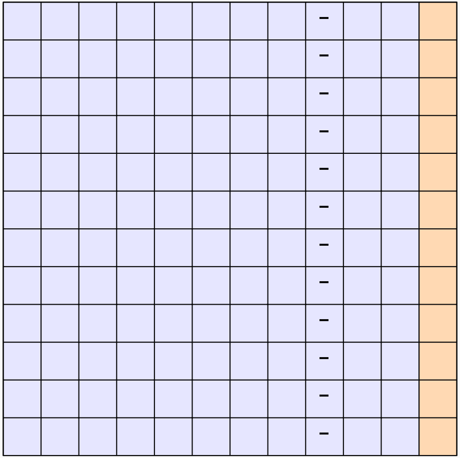

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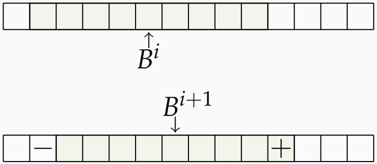

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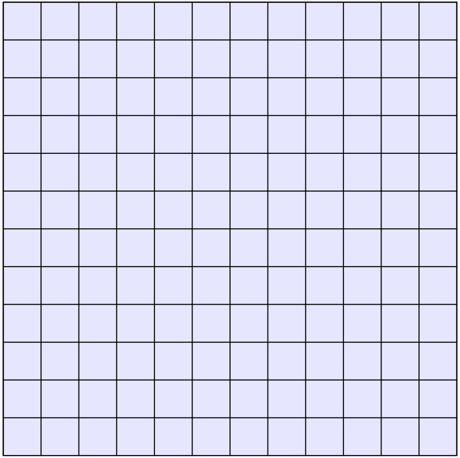
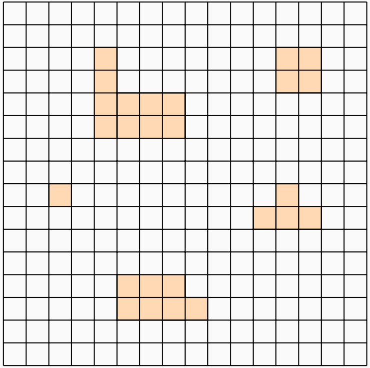
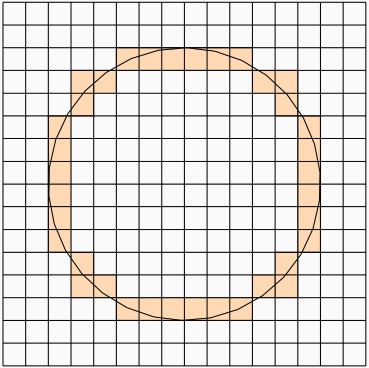


GLOBAL SWEEP: DRAWBACKS

Sparse Volume distribution



Surface Distribution



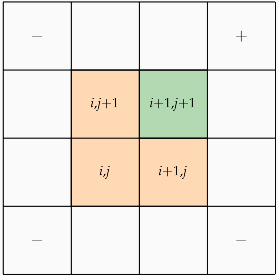
Global sweep *fills-in* empty boxes

Higher storage and compuational costs

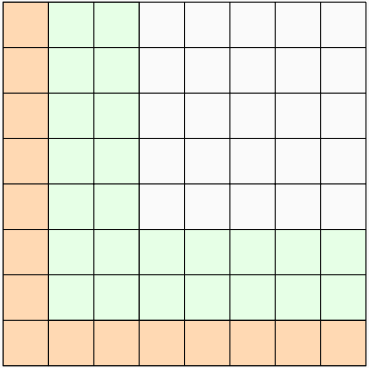
New Stencil

$$v_k^{(i+1,j+1)} = \sum_{\xi} (-1)^{1+d+\mathcal{M}(\xi)} e^{i\lambda k\cdot\xi} v_k^{(i,j)+\xi}$$

$$+ \sum_{\chi} (-1)^{1+d+\mathcal{M}(\chi)} e^{i\lambda k\cdot\chi} w_k^{(i,j)+\chi}.$$



Direct translation for first layer



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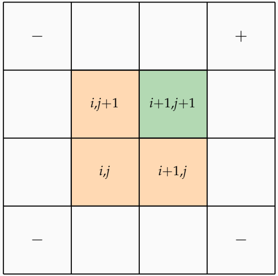
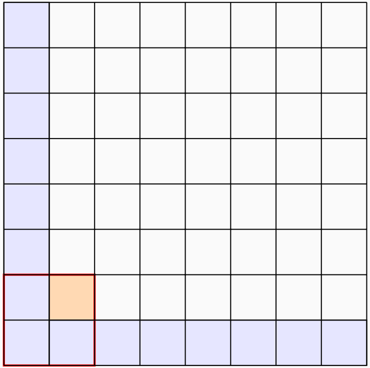


Propagate to subsequent layers



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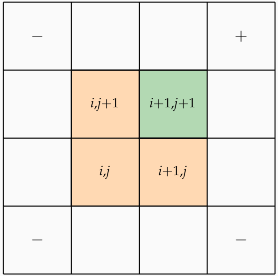

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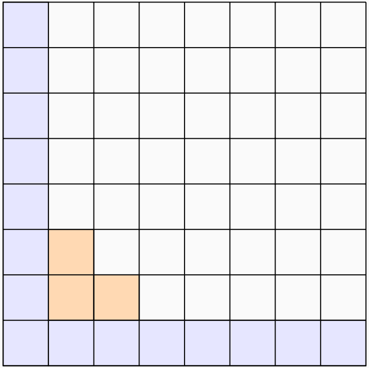

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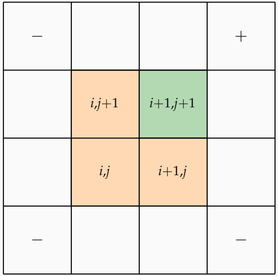

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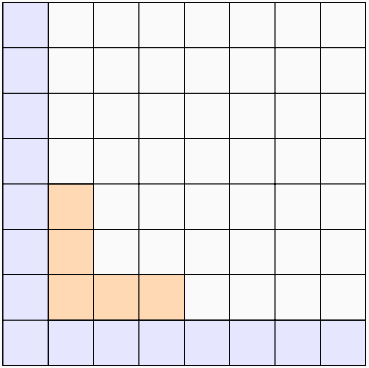

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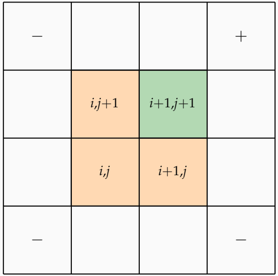

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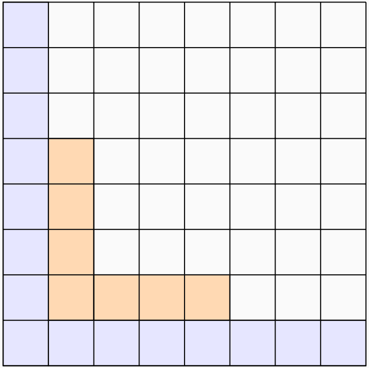

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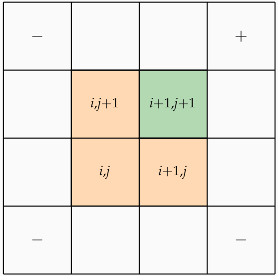

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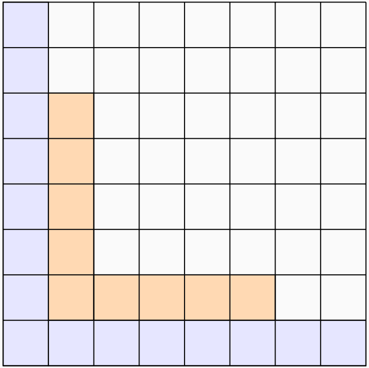

New Stencil

$$v_k^{(i+1,j+1)} = \sum_{\xi} (-1)^{1+d+\mathcal{M}(\xi)} e^{i\lambda k\cdot\xi} v_k^{(i,j)+\xi}$$

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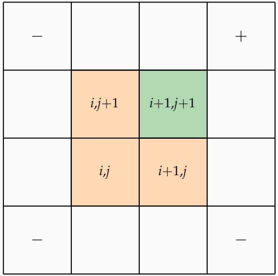

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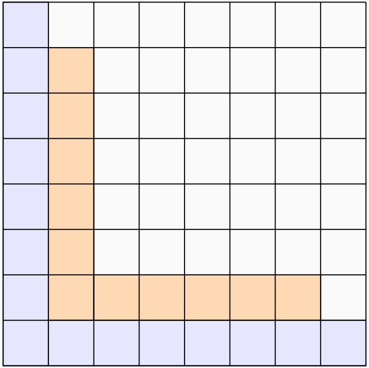

VOLUME DISTRIBUTIONS: LOCAL SWEEP

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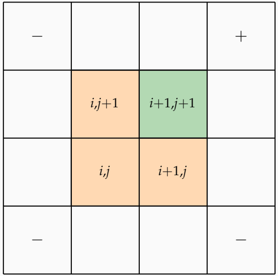

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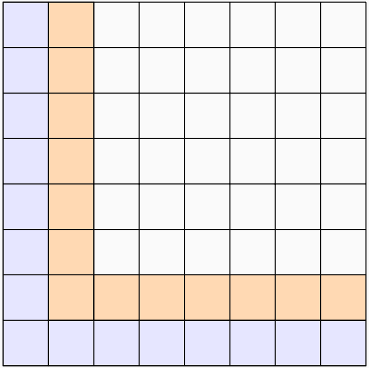

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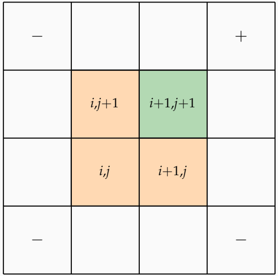

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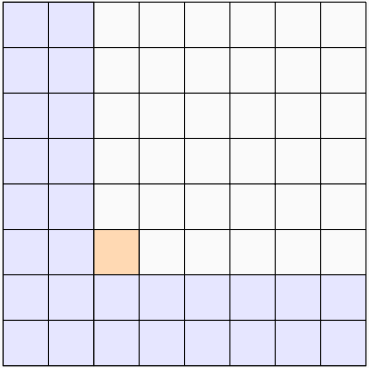

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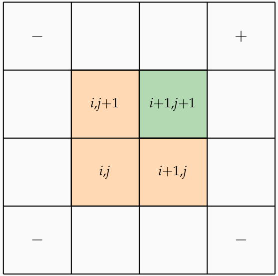

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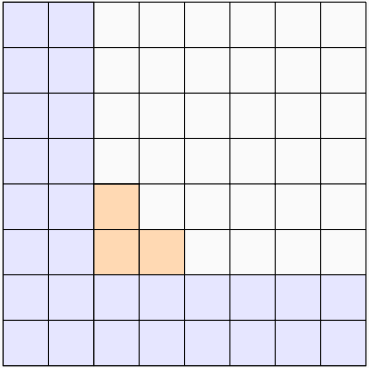

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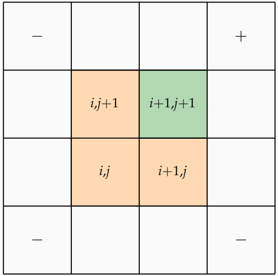

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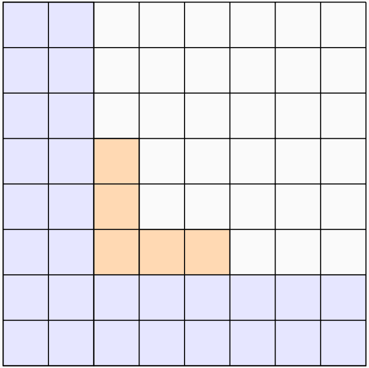

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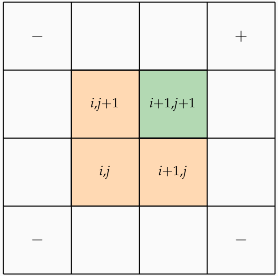

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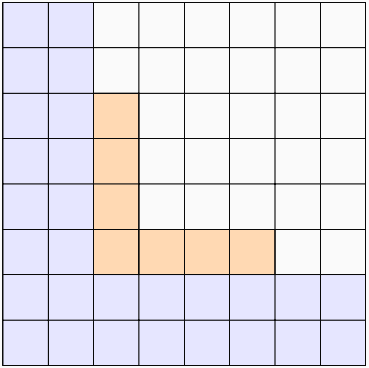

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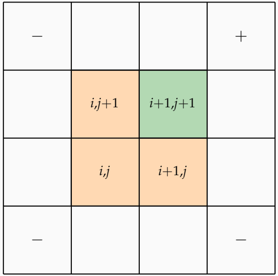

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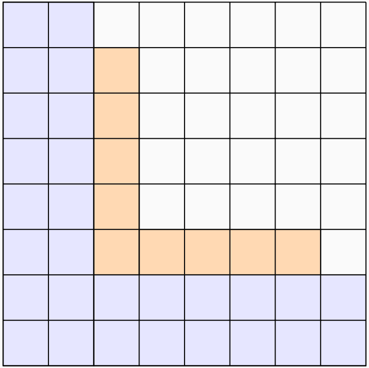

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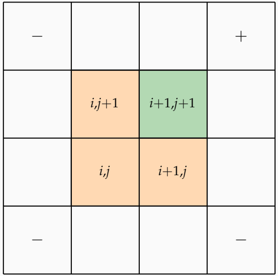

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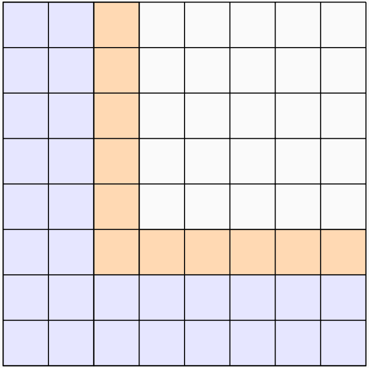

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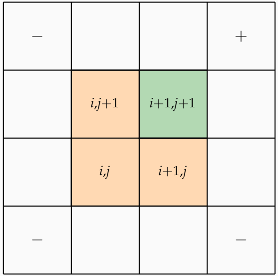

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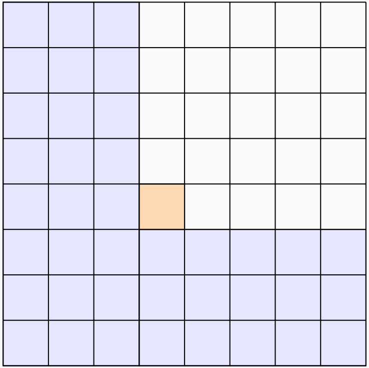

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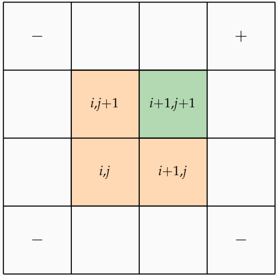

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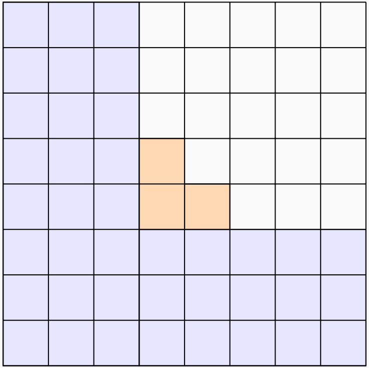

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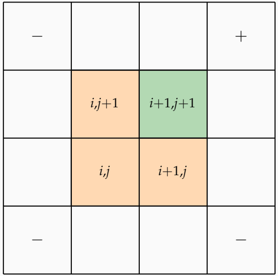

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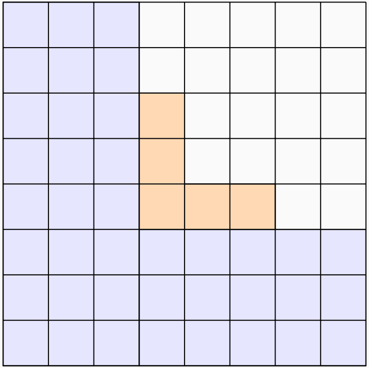

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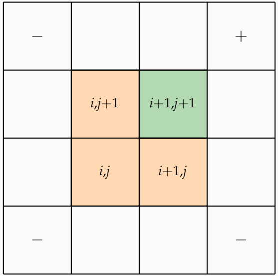

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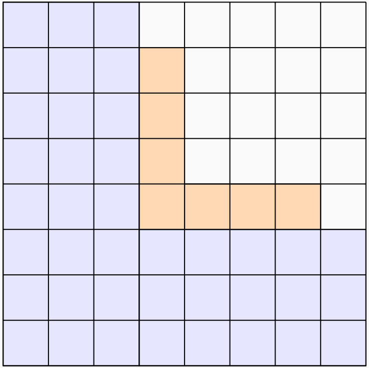

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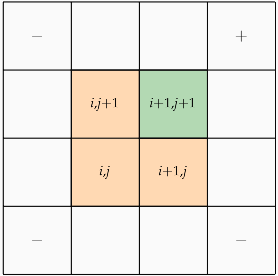

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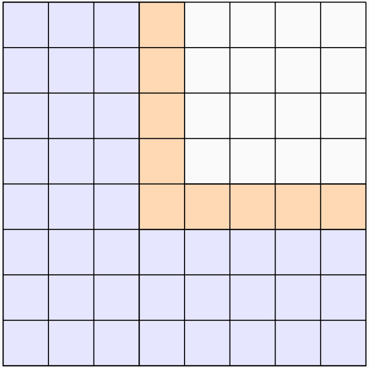

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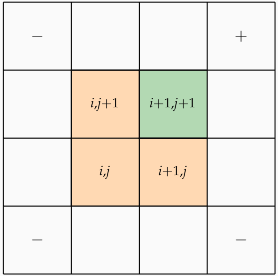

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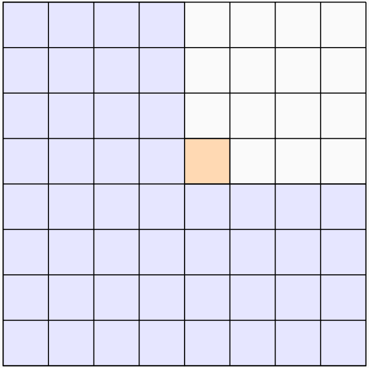

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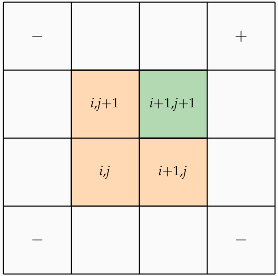

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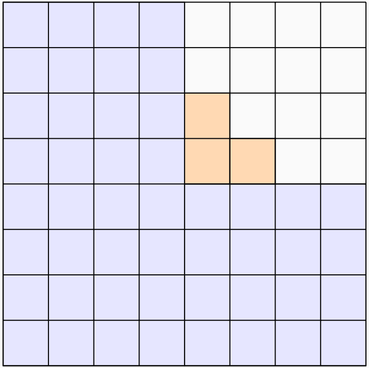

VOLUME DISTRIBUTIONS: LOCAL SWEEP

New Stencil

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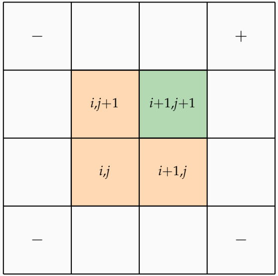

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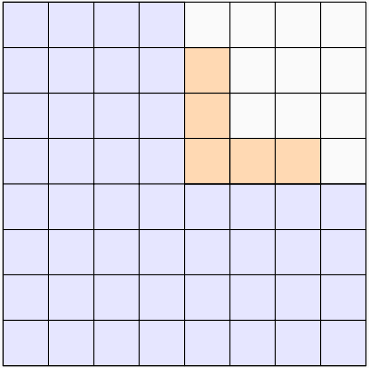

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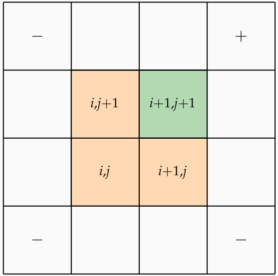

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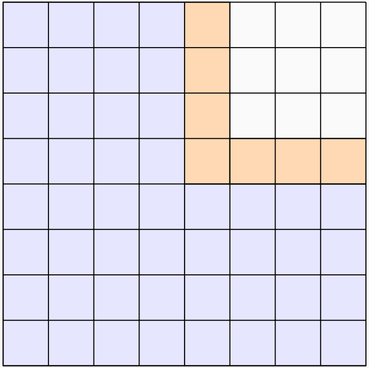

VOLUME DISTRIBUTIONS: LOCAL SWEEP

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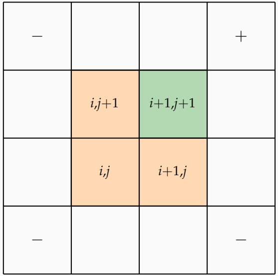

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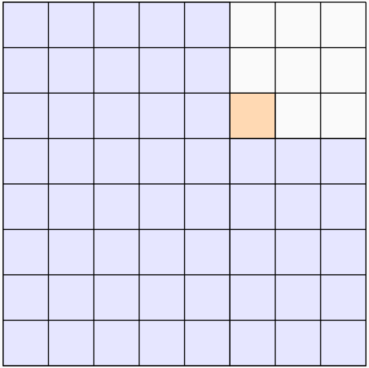

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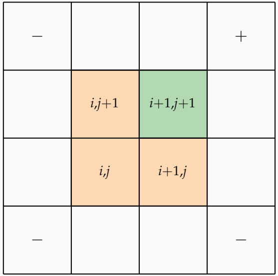

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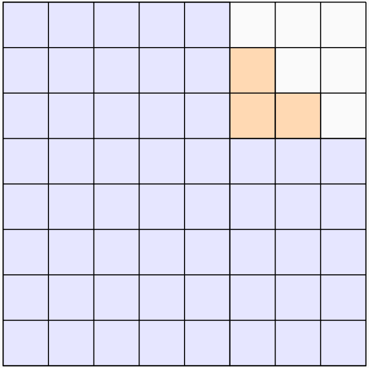

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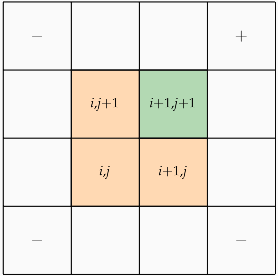

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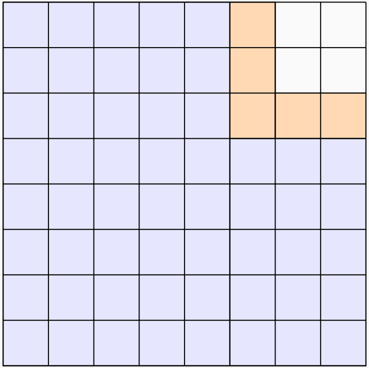

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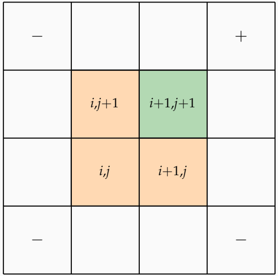

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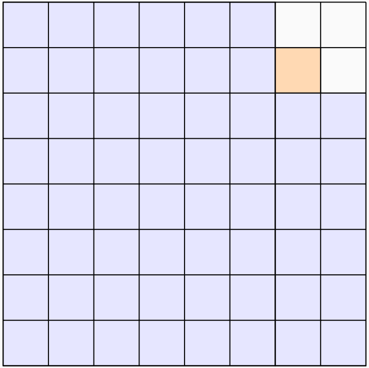

VOLUME DISTRIBUTIONS: LOCAL SWEEP

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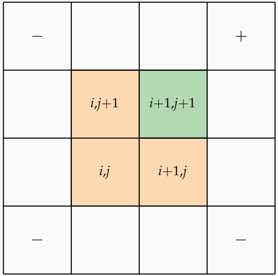

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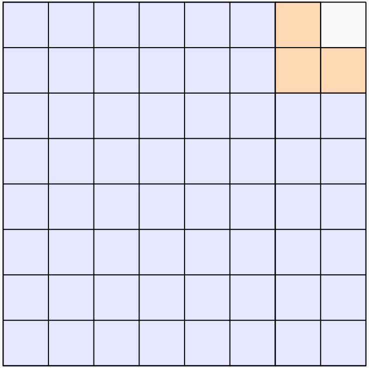

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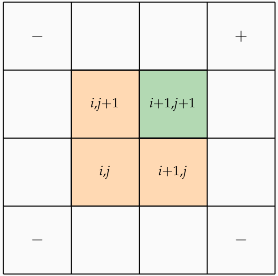

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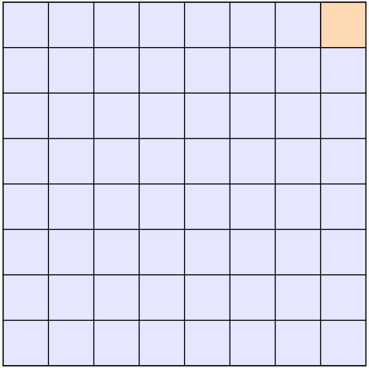

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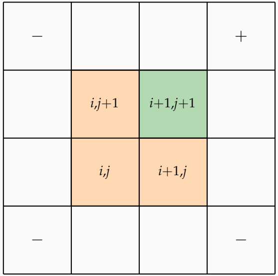

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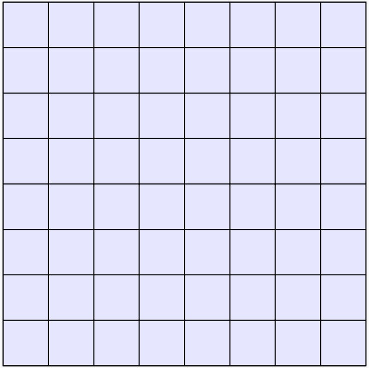
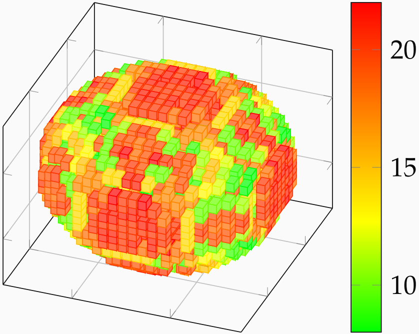


Find an ordering that maximizes overlap of consecutive interaction lists

reduce to finding a *minimum spanning tree*

use Kruskal's algorithm

$\mathcal{O}(K^2 p^3) \to \mathcal{O}(K p^3)$



MST - RESULTS

$$K = 9, \epsilon = 10^{-6}$$

$\|B\|$	direct	MST	ratio
$1K$	$114K$	$18K$	6.3
$10K$	$1M$	$182K$	5.88
$100K$	$9.65M$	$1.7M$	5.68
$1M$	$96.8M$	$17.1M$	5.68

MST - RESULTS

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$$K = 13, \epsilon = 10^{-12}$$

$\lvert B \rvert$	direct	MST	ratio
$1K$	$238K$	$24K$	9.65
$10K$	$2.2M$	$264K$	8.48
$100K$	$20.2M$	$2.5M$	8.18
$1M$	$200.6M$	$24.5M$	8.18

Nonuniform Distributions

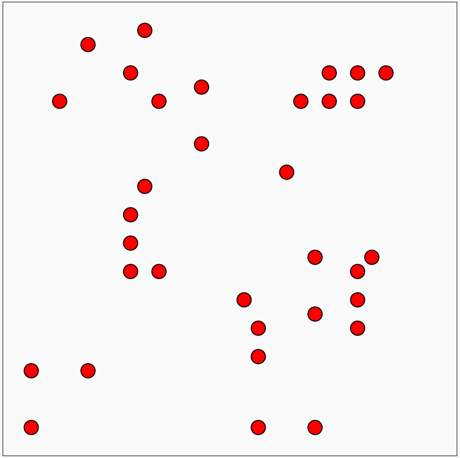
EXPANSION OR TRUNCATION?

Many sources per FGT box – Expansion

Few sources per FGT box – Truncation

Non-uniform distributions – Hybrid

Max. of m points per leaf

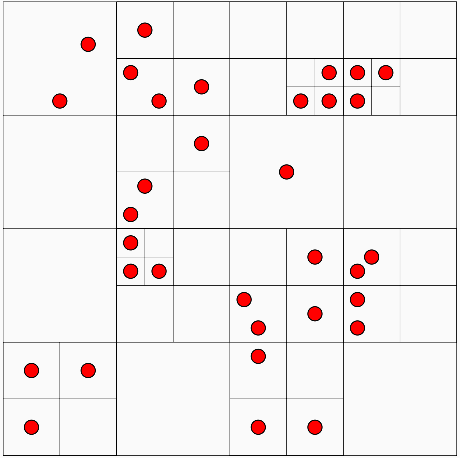


$m = 2$

TREE CONSTRUCTION

Max. of m points per leaf

Higher point density $\Rightarrow$ finer leaves



$m = 2$

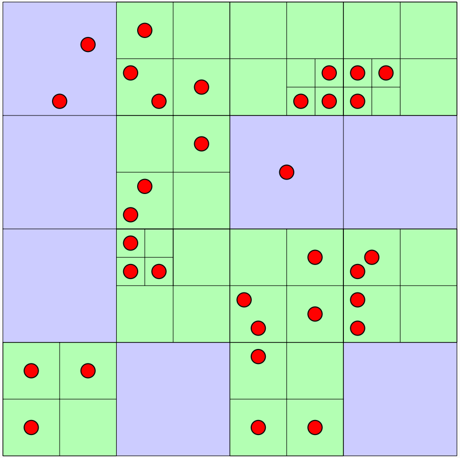
TREE CONSTRUCTION

Max. of m points per leaf

Higher point density $\Rightarrow$ finer leaves

Large leaves $\Rightarrow$ Truncation (Direct)

Small leaves $\Rightarrow$ Expansion (Expand)



$m = 2$

FLOW OF INFORMATION

Source — y

Target — x

Direct tree — T_d

Expand tree — T_e

$$
\begin{array}{ccl}
y & x & \\
T_e & T_e & y \xrightarrow{\textbf{S2W}} \{w_k\} \xrightarrow{\textbf{W2L}} \{v_k\} \xrightarrow{\textbf{L2T}} x \\
T_e & T_d & y \xrightarrow{\textbf{S2W}} \{w_k\} \xrightarrow{\qquad\textbf{W2D}\qquad} x \\
T_d & T_e & y \xrightarrow{\qquad\textbf{D2L}\qquad} \{v_k\} \xrightarrow{\textbf{L2T}} x \\
T_d & T_d & y \xrightarrow{\qquad\qquad\textbf{D2D}\qquad\qquad} x
\end{array}
$$

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Source — y

Target — x

Direct tree — T_d

Expand tree — T_e

$$F(x) += \sum_{|k|\leq p} \hat{G}(k) w_k e^{i\lambda k\cdot(x-c^B)}$$

y	x	
T_e	T_e	$y \xrightarrow{\text{S2W}} \{w_k\} \xrightarrow{\text{W2L}} \{v_k\} \xrightarrow{\text{L2T}} x$
T_e	T_d	$y \xrightarrow{\text{S2W}} \{w_k\} \xrightarrow{\text{W2D}} x$
T_d	T_e	$y \xrightarrow{\text{D2L}} \{v_k\} \xrightarrow{\text{L2T}} x$
T_d	T_d	$y \xrightarrow{\text{D2D}} x$

FLOW OF INFORMATION

Source — y

Target — x

Direct tree — T_d

Expand tree — T_e

$$v_k + = f(y) e^{i\lambda k \cdot (c^D - y)}$$

y	x	
T_e	T_e	$y \xrightarrow{\textbf{S2W}} \{w_k\} \xrightarrow{\textbf{W2L}} \{v_k\} \xrightarrow{\textbf{L2T}} x$
T_e	T_d	$y \xrightarrow{\textbf{S2W}} \{w_k\} \xrightarrow{\textbf{W2D}} x$
T_d	T_e	$y \xrightarrow{\textbf{D2L}} \{v_k\} \xrightarrow{\textbf{L2T}} x$
T_d	T_d	$y \xrightarrow{\textbf{D2D}} x$

FLOW OF INFORMATION

Source — y

Target — x

Direct tree — T_d

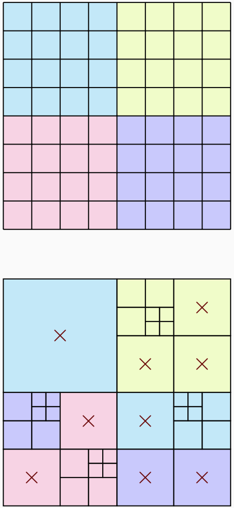
Expand tree — T_e

$$F(x) += G_\delta(\|x-y\|)f(y)$$

$$
\begin{array}{cccl}
y & x & & \\
T_e & T_e & y & \xrightarrow{\textbf{S2W}} \{w_k\} \xrightarrow{\textbf{W2L}} \{v_k\} \xrightarrow{\textbf{L2T}} x \\
T_e & T_d & y & \xrightarrow{\textbf{S2W}} \{w_k\} \xrightarrow{\textbf{W2D}} x \\
T_d & T_e & y & \xrightarrow{\textbf{D2L}} \{v_k\} \xrightarrow{\textbf{L2T}} x \\
T_d & T_d & y & \xrightarrow{\textbf{D2D}} x
\end{array}
$$

DATA PARTITION

- Distributed regular grid of FGT boxes
  - Each box owned by an unique CPU
  - Each CPU owns a sub-grid of boxes
  - PETSc package
- Distributed octree
  - Each leaf owned by an unique CPU
  - Sorted in Morton (space-filling) order
  - Direct and Expand trees partitioned independently
  - Dendro package
- Distributed points — mapped to enclosing leaf



PARALLEL ALGORITHM

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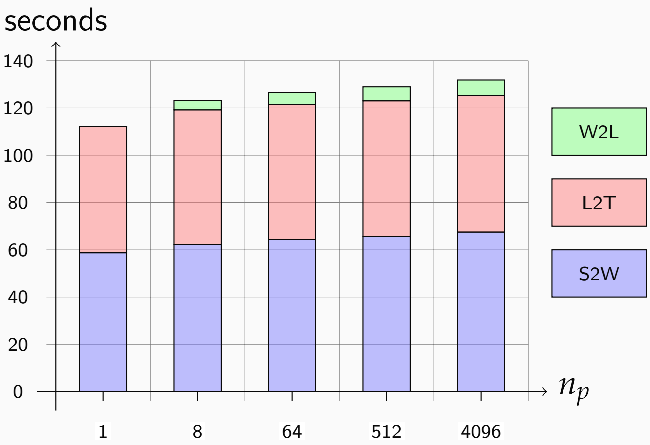
Step	Computation	Communication
S2W	Compute wave expansions for Expand sources	Send wave expansions to FGT boxes
W2D	Update transform at Direct targets	Send wave expansions to Direct targets
D2D	Update transform at Direct targets	Send Direct sources to Direct targets
W2L	Execute translation/sweeping algorithm	Communicate wave expansions of *ghost* FGT boxes
D2L	Update local expansions of FGT boxes using contributions from Direct sources	Send contributions from Direct sources to FGT boxes
L2T	Compute transform at Expand targets	Send local expansions to Expand targets

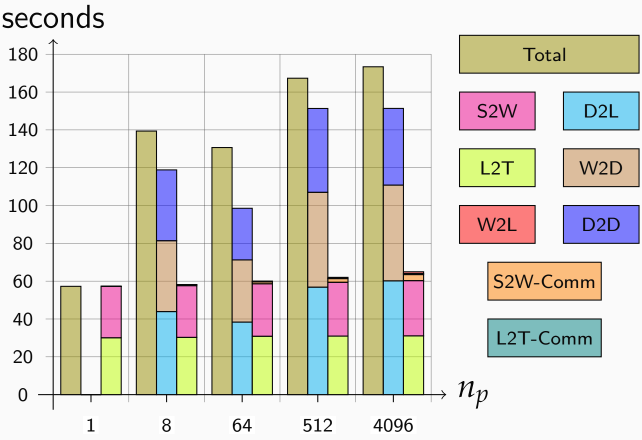
Results

ISOGRANULAR SCALABILITY - UNIFORM



≈ 30M Points/CPU

ISOGRANULAR SCALABILITY - GAUSSIAN



≈ 300K Points/CPU

SUMMARY

A novel translation scheme

- lower computational and storage costs

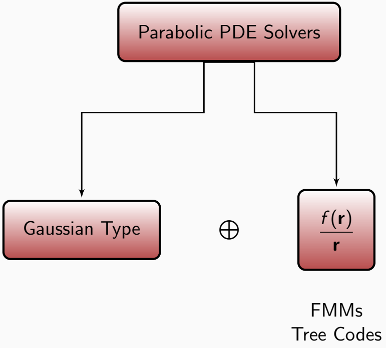
A novel octree-based algorithm for highly nonuniform distributions

- optimal in all ranges of δ

Massively parallel algorithm for nonuniform distributions

- excellent scalability

Supports any Gaussian-type kernel



FUTURE WORK

Reducing the constants

- Hermite to plane-wave conversion
- Overlap communication with computation

Code release under GNU -GPL `github.com/paralab/pgft`

Additional machinery required for *black-box* integral equation solvers for general parabolic PDEs

Questions?