6.506: Algorithm Engineering

Lecture 5 (Stencil Computations)

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What is a Stencil Computation?



Space N

We are given spatial (input) grid data a_0 at time 0.

A stencil S computes a cell value in a spatial grid a_t at time t from nearby values at times before t.

A stencil computation applies S to a_o for a given T number of timesteps to compute the output grid a_T .

Examples of Stencils







Example: 2D Heat Diffusion

Let $h_t(x, y)$ be the heat at point (x, y) at time t.

Heat Equation

$$\frac{\partial h}{\partial t} = \alpha \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right), \ \alpha = \text{thermal diffusivity}$$

Update Equation (on a discrete grid)

$$h_{t+1}(x,y) = h_t(x,y) + c_x (h_t(x+1,y) - 2h_t(x,y) + h_t(x-1,y)) + c_y (h_t(x,y+1) - 2h_t(x,y) + h_t(x,y-1))$$

2D 5-point Stencil







Stencil Applications



Fluid Dynamics



Mechanical Engg.







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Meteorology

Image Processing

ing Cellular Automata

Standard $\Theta(NT)$ Work Stencil Algorithms





Space N

Implementation Trick: Reuse storage for odd and even time steps

```
for t \leftarrow 1 to T do
    k \leftarrow t \mod 2
    for i \leftarrow 0 to N - 1 do
        compute a_k[i] from a_{1-k}
        using the stencil
```





Work: Computes each of the TN cells exactly once in $\Theta(1)$ time.

Total work, $T_1(T, N) = \Theta(TN)$

Span: In each time step computes all N cells in parallel.

Total span, $T_{\infty}(T, N) = \Theta(T \log N)$





Space N

Serial Cache Complexity: It performs T sequential scans of a_0 and a_1 .

Serial cache complexity, $Q_1(T, N) = O\left(\frac{TN}{B}\right)$,

where, B = cache line size.

Implementation Tricks

- Reuse storage for odd and even time steps
- Keep a halo of ghost cells around the array with boundary values





Cache-optimized version of the standard looping code.

The computation proceeds in **blocks/tiles** to achieve temporal data locality.

Cache-aware: cache size *M* must be known for blocking.

Code generators: PLuTo, Devito, etc.







- N ·

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Each grid cell is computed exactly once in $\Theta(1)$ work.

Total work, $T_1(T, N) = \Theta(TN)$







The algorithm exploits data locality cache-obliviously through recursive tiling.

Code generator: Pochoir (MIT/Fudan/SBU)

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In grids of spatial dimension ≥ 2 , a hyperspace cut simultaneously cuts as many spatial dimensions as possible.

All 3^k subtrapezoids created by a hyperspace cut on $k \ge 1$ of the $d \ge k$ spatial dimensions of a (d + 1)-dimensional trapezoid can be evaluated in k + 1 parallel steps.

Recent o(NT) Work Stencil Algorithms

Theoretical Results

N: #cells in the spatial grid, **T**: #timesteps

Algorithm	Work	Span
Nested Loop		$\Theta(T\log N)$
Tiled Loop	$\Theta(NT)$	$\Theta\left(T\log M + \frac{T}{M^{1/d}}\log\frac{N}{M}\right)$
Recursive Tiling (Trapezoidal Decomp)		$\Theta\left(T\left(N^{1/d}\right)^{\log_2(d+2)-1}\right)$
FFT-Periodic (SPAA'21)	$\Theta(N \log(NT))$	$\Theta(\log T + \log N \log \log N)$
FFT-Aperiodic (SPAA'21)	$\Theta\left(TN^{1-\frac{1}{d}}\log\left(TN^{1-\frac{1}{d}}\right)\log T + N\log N\right)$	$\Theta(T)$ if $d = 1$ $\Theta(T \log N)$ if $d \ge 2$
Gaussian-Freespace (SPAA'22)	$\Theta\left(N\log^{O(d)}\left(\frac{1}{\epsilon}\right) + \log T\right)$	$\Theta\left(\log N \log^{O(d)}\left(\frac{1}{\epsilon}\right) + \log T\right)$

d: dimension of the spatial grid, M: tile size , ϵ : additive error

Applicability of the New Algorithms



KNL (Intel Knight's Landing): 68 cores, SKX (Intel Skylake): 48 cores

PLuTo: State-of-the-art Tiled Looping Code Generator for Multicores

Ber	nchma	ark			Parallel runtime in seconds				Speedup factor		
					PLu	ıTo	Our alg	gorithm	over F	LuTo	
		Stencil	N	Т	KNL	SKX	KNL	SKX	KNL	SKX	
		heat1d	1,600,000	10^{6}	79	19	0.25	0.03	1754.7	759.6	
	C	heat2d	$8,000 \times 8,000$	10^{5}	1,437	222	0.48	0.61	3,025.0	367.0	
	ipol	seidel2d	$8,000 \times 8,000$	10^{5}	500	808	0.48	0.64	1,032.7	1268.6	
	Per	jacobi2d	$8,000 \times 8,000$	10^{5}	2,905	1017	0.48	0.68	6,084.7	1502.1	
		heat3d	$800 \times 800 \times 800$	10^{4}	816	1466	4.98	5.48	163.9	267.3	
		19pt3d	$800 \times 800 \times 800$	10^{4}	141	158	4.84	5.78	29.1	27.3	
		heat1d	1,600,000	10^{6}	50	35	5.85	6.69	8.5	5.2	
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lic	ExJ	heat3d	$800 \times 800 \times 800$	10^{4}	513	763	395.10	605.89	1.3	1.3	
rioc		19pt3d	$800 \times 800 \times 800$	10^{4}	645	848	425.22	616.71	1.5	1.4	
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		Stencil	N	Т	KNL	SKX	KNL	SKX	KNL	SKX
		heat1d	1,600,000	10^{6}	79	19	0.25	0.03	1754.7	759.6
	C	heat2d	$8,000 \times 8,000$	10^{5}	1,437	222	0.48	0.61	3,025.0	367.0
	1001	seidel2d	$8,000 \times 8,000$	10^{5}	500	808	0.48	0.64	1,032.7	1268.6
	rer	jacobi2d	$8,000 \times 8,000$	10^{5}	2,905	1017	0.48	0.68	6,084.7	1502.1
		heat3d	$800 \times 800 \times 800$	10^{4}	816	1466	4.98	5.48	163.9	267.3
		19pt3d	$800 \times 800 \times 800$	10^{4}	141	158	4.84	5.78	29.1	27.3
	1	heat1d	1,600,000	10^{6}	50	35	5.85	6.69	8.5	5.2
	nt	heat2d	$8,000 \times 8,000$	10^{5}	333	530	143.25	151.37	2.3	3.5
	ime	seidel2d	$8,000 \times 8,000$	10^{5}	345	601	145.42	132.97	2.4	4.5
	per	jacobi2d	$8,000 \times 8,000$	10^{5}	567	456	249.04	273.46	2.3	1.7
lic	ExJ	heat3d	$800 \times 800 \times 800$	10^{4}	513	763	395.10	605.89	1.3	1.3
rioc		19pt3d	$800 \times 800 \times 800$	10^{4}	645	848	425.22	616.71	1.5	1.4
Ape	2	heat1d	1,600,000	N_{-}	32	23	5.63	6.87	5.7	3.3
	ant	heat2d	$8,000 \times 8,000$	\sqrt{N}	210	312	92.78	121.70	2.3	2.6
	ime	seidel2d	$8,000 \times 8,000$	\sqrt{N}	228	375	91.59	121.46	2.5	3.1
	per	jacobi2d	$8,000 \times 8,000$	\sqrt{N}	372	281	151.31	198.00	2.5	1.4
	Ex	heat3d	$800 \times 800 \times 800$	$\sqrt[3]{N}$	45	71	32.29	50.52	1.4	1.4
		19pt3d	$800 \times 800 \times 800$	$\sqrt[3]{N}$	61	71	33.82	52.27	1.8	1.4

Some Performance Numbers (Periodic)

KNL (Intel Knight's Landing): 68 cores, SKX (Intel Skylake): 48 cores

PLuTo: State-of-the-art Tiled Looping Code Generator for Multicores



Some Performance Numbers (Aperiodic, $T = N^{1/d}$)

KNL (Intel Knight's Landing): 68 cores, SKX (Intel Skylake): 48 cores

PLuTo: State-of-the-art Tiled Looping Code Generator for Multicores Intel MKL was used for FFT Implementations



Some Performance Numbers (Aperiodic, $T = N^{1/d}$)

KNL (Intel Knight's Landing): 68 cores, SKX (Intel Skylake): 48 cores

PLuTo: State-of-the-art Tiled Looping Code Generator for Multicores



cores: <u>48</u> (24 / socket)

SKX (Intel Skylake)

caches: 32 KB L1 / core, 1 MB L2 / core, 33 MB L3 / socket RAM: 192 GB DDR4

Stencil	N	T	Runn	ing Time (s	ec)	Error (w.r.t. FFT)				
Stencii	IV	1	Gaussian	PLuTo	FFT	Mean Squared				
		10 ³	0.10	0.49	0.02					
		104	0.11	2.10	0.02					
heat 1d (3 pt)	1.6×10^{6}	10 ⁵	0.11	8.73	0.02					
		106	0.11	217.56	0.04					
		107	0.10	> 10 m	0.32	1.57×10^{-14}				
		10 ³	0.45	1.58	0.08					
heat 2d (5 pt)	1000 imes 1000	104	0.42	53.74	4.55					
		10 ⁵	0.15	out of me	mory					
		10 ³	0.40	2.41	0.08					
Seidel 2d (9 pt)	1000 imes 1000	104	0.40	567.46	5.59					
() ()		10 ⁵	0.15	out of me	mory					
Jacobi 2d	1000 × 1000	10 ³	0.60	4.24	0.22					
(25 pt)	1000 × 1000	104	0.51	out of me	mory					
heat 3d	$100 \times 100 \times 100$	10 ^{2.7}	10.35	271.52	11.81					
(7 pt)	100 × 100 × 100	10 ³	3.31	out of me	mory					

cores: <u>48</u> (24 / socket)

SKX (Intel Skylake)

caches: 32 KB L1 / core, 1 MB L2 / core, 33 MB L3 / socket RAM: 192 GB DDR4

Stencil	N	T	Runn	ing Time (s	ec)	Error (w.r.t. FFT)				
Stencii	11	1	Gaussian	PLuTo	FFT	Mean Squared				
		10 ³	0.10	0.49	0.02	1.13×10^{-12}				
		104	0.11	2.10	0.02	2.01×10^{-13}				
heat 1d (3 pt)	1.6×10^{6}	10 ⁵	0.11	8.73	0.02	3.58×10^{-14}				
		10 ⁶	0.11	217.56	0.04	6.44×10^{-15}				
		107	0.10	> 10 m	0.32	1.57×10^{-14}				
		10 ³	0.45	1.58	0.08	7.29×10^{-11}				
heat 2d (5 pt)	1000×1000	104	0.42	53.74	4.55	3.12×10^{-11}				
		10 ⁵	0.15	out of me	emory					
		10 ³	0.40	2.41	0.08	1.23×10^{-10}				
Seidel 2d (9 pt)	1000×1000	104	0.40	567.46	5.59	2.13×10^{-11}				
() ()		10 ⁵	0.15	out of me	emory					
Jacobi 2d	1000 × 1000	10 ³	0.60	4.24	0.22	1.30×10^{-7}				
(25 pt)	1000 × 1000	104	0.51	out of me	emory					
heat 3d	$100 \times 100 \times 100$	10 ^{2.7}	10.35	271.52	11.81	2.21×10^{-10}				
(7 pt)	100 × 100 × 100	10 ³	3.31	out of me	emory					

cores: <u>48</u> (24 / socket)

SKX (Intel Skylake)

caches: 32 KB L1 / core, 1 MB L2 / core, 33 MB L3 / socket RAM: 192 GB DDR4

Stencilheat 1d (3 pt)heat 2d (5 pt)Seidel 2d (9 pt)Jacobi 2d (25 pt)heat 3d (7 pt)10	N	T	Runn	ing Time (s	ec)	Error (w.r.t. FFT)				
	IV	1	Gaussian	PLuTo	FFT	Mean Squared	Max Absolute	Mean Relative	Max Relative	
		10 ³	0.10	0.49	0.02	1.13×10^{-12}	2.29×10^{-10}	1.20×10^{-9}	3.03×10^{-5}	
		104	0.11	2.10	0.02	2.01×10^{-13}	2.29×10^{-11}	5.27×10^{-10}	3.03×10^{-6}	
heat 1d (3 pt)	1.6×10^{6}	10 ⁵	0.11	8.73	0.02	3.58×10^{-14}	2.29×10^{-12}	2.50×10^{-10}	3.03×10^{-7}	
(10 ⁶	0.11	217.56	0.04	6.44×10^{-15}	2.30×10^{-13}	1.15×10^{-10}	3.05×10^{-8}	
		107	0.10	> 10 m	0.32	1.57×10^{-14}	5.03×10^{-14}	1.41×10^{-9}	6.74×10^{-9}	
		10 ³	0.45	1.58	0.08	7.29×10^{-11}	3.34×10^{-10}	5.91×10^{-6}		
heat 2d (5 pt)	1000 imes 1000	10 ⁴	0.42	53.74	4.55	3.12×10^{-11}				
		10 ⁵	0.15	out of me	mory					
		10 ³	0.40	2.41	0.08	1.23×10^{-10}				
Seidel 2d (9 pt)	1000 imes 1000	10 ⁴	0.40	567.46	5.59	2.13×10^{-11}				
		10 ⁵	0.15	out of me	mory					
Jacobi 2d	1000 × 1000	10 ³	0.60	4.24	0.22	1.30×10^{-7}				
(25 pt)	1000 × 1000	104	0.51	out of me	mory					
heat 3d	100 × 100 × 100	10 ^{2.7}	10.35	271.52	11.81	2.21×10^{-10}				
(7 pt)	100 × 100 × 100	10 ³	3.31	out of me	mory					

cores: <u>48</u> (24 / socket)

SKX (Intel Skylake)

caches: 32 KB L1 / core, 1 MB L2 / core, 33 MB L3 / socket RAM: 192 GB DDR4

Stoneil	N	T	Runn	ing Time (s	ec)		Error (w	.r.t. FFT)	
Stencii	IV	1	Gaussian	PLuTo	FFT	Mean Squared	Max Absolute	Mean Relative	Max Relative
		10 ³	0.10	0.49	0.02	1.13×10^{-12}	2.29×10^{-10}	1.20×10^{-9}	3.03×10^{-5}
		104	0.11	2.10	0.02	2.01×10^{-13}	2.29×10^{-11}	5.27×10^{-10}	3.03×10^{-6}
heat 1d (3 pt)	1.6×10^{6}	10 ⁵	0.11	8.73	0.02	3.58×10^{-14}	2.29×10^{-12}	2.50×10^{-10}	3.03×10^{-7}
		10 ⁶	0.11	217.56	0.04	6.44×10^{-15}	2.30×10^{-13}	1.15×10^{-10}	3.05×10^{-8}
		107	0.10	> 10 m	0.32	1.57×10^{-14}	5.03×10^{-14}	1.41×10^{-9}	6.74×10^{-9}
		10 ³	0.45	1.58	0.08	7.29×10^{-11}	3.34×10^{-10}	5.91×10^{-6}	6.36×10^{-5}
heat 2d (5 pt)	1000×1000	10 ⁴	0.42	53.74	4.55	3.12×10^{-11}	4.22×10^{-11}	3.41×10^{-6}	6.30×10^{-6}
		10 ⁵	0.15				out of memory		
		10 ³	0.40	2.41	0.08	1.23×10^{-10}	5.31×10^{-10}	1.19×10^{-5}	
Seidel 2d (9 pt)	1000 imes 1000	104	0.40	567.46	5.59	2.13×10^{-11}			
		10 ⁵	0.15	out of me	emory				
Jacobi 2d	1000 × 1000	10 ³	0.60	4.24	0.22	1.30×10^{-7}			
(25 pt)	1000 × 1000	104	0.51	out of me	emory				
heat 3d	$100 \times 100 \times 100$	10 ^{2.7}	10.35	271.52	11.81	2.21×10^{-10}			
(7 pt)	100 × 100 × 100	10 ³	3.31	out of me	emory				

cores: <u>48</u> (24 / socket)

SKX (Intel Skylake)

caches: 32 KB L1 / core, 1 MB L2 / core, 33 MB L3 / socket RAM: 192 GB DDR4

Stencil	Ν	Т	Running Time (sec)			Error (w.r.t. FFT)				
			Gaussian	PLuTo	FFT	Mean Squared	Max Absolute	Mean Relative	Max Relative	
heat 1d (3 pt)	1.6×10^{6}	10 ³	0.10	0.49	0.02	1.13×10^{-12}	2.29×10^{-10}	1.20×10^{-9}	3.03×10^{-5}	
		10 ⁴	0.11	2.10	0.02	2.01×10^{-13}	2.29×10^{-11}	5.27×10^{-10}	3.03×10^{-6}	
		10 ⁵	0.11	8.73	0.02	3.58×10^{-14}	2.29×10^{-12}	2.50×10^{-10}	3.03×10^{-7}	
		10 ⁶	0.11	217.56	0.04	6.44×10^{-15}	2.30×10^{-13}	1.15×10^{-10}	3.05×10^{-8}	
		10 ⁷	0.10	> 10 m	0.32	1.57×10^{-14}	5.03×10^{-14}	1.41×10^{-9}	6.74×10^{-9}	
heat 2d (5 pt)	1000 × 1000	10 ³	0.45	1.58	0.08	7.29×10^{-11}	3.34×10^{-10}	5.91×10^{-6}	6.36×10^{-5}	
		10 ⁴	0.42	53.74	4.55	3.12×10^{-11}	4.22×10^{-11}	3.41×10^{-6}	6.30×10^{-6}	
		10 ⁵	0.15	out of memory						
Seidel 2d (9 pt)	1000×1000	10 ³	0.40	2.41	0.08	1.23×10^{-10}	5.31×10^{-10}	1.19×10^{-5}	9.36×10^{-5}	
		10 ⁴	0.40	567.46	5.59	2.13×10^{-11}	6.12×10^{-11}	2.14×10^{-6}	8.72×10^{-6}	
		10 ⁵	0.15	out of memory						
Jacobi 2d (25 pt)	1000×1000	10 ³	0.60	4.24	0.22	1.30×10^{-7}	1.61×10^{-7}	1.35×10^{-2}	2.08×10^{-2}	
		104	0.51	out of memory						
heat 3d (7 pt)	$100 \times 100 \times 100$	10 ^{2.7}	10.35	271.52	11.81	2.21×10^{-10}				
		10 ³	3.31	out of memory						

cores: <u>48</u> (24 / socket)

SKX (Intel Skylake)

caches: 32 KB L1 / core, 1 MB L2 / core, 33 MB L3 / socket RAM: 192 GB DDR4

Stencil	Ν	Т	Running Time (sec)			Error (w.r.t. FFT)				
			Gaussian	PLuTo	FFT	Mean Squared	Max Absolute	Mean Relative	Max Relative	
heat 1d (3 pt)	1.6×10^{6}	10 ³	0.10	0.49	0.02	1.13×10^{-12}	2.29×10^{-10}	1.20×10^{-9}	3.03×10^{-5}	
		10 ⁴	0.11	2.10	0.02	2.01×10^{-13}	2.29×10^{-11}	5.27×10^{-10}	3.03×10^{-6}	
		10 ⁵	0.11	8.73	0.02	3.58×10^{-14}	2.29×10^{-12}	2.50×10^{-10}	3.03×10^{-7}	
		10 ⁶	0.11	217.56	0.04	6.44×10^{-15}	2.30×10^{-13}	1.15×10^{-10}	3.05×10^{-8}	
		107	0.10	> 10 m	0.32	1.57×10^{-14}	5.03×10^{-14}	1.41×10^{-9}	6.74×10^{-9}	
heat 2d (5 pt)	1000 × 1000	10 ³	0.45	1.58	0.08	7.29×10^{-11}	3.34×10^{-10}	5.91×10^{-6}	6.36×10^{-5}	
		10 ⁴	0.42	53.74	4.55	3.12×10^{-11}	4.22×10^{-11}	3.41×10^{-6}	6.30×10^{-6}	
		10 ⁵	0.15	out of memory						
Seidel 2d (9 pt)	1000×1000	10 ³	0.40	2.41	0.08	1.23×10^{-10}	5.31×10^{-10}	1.19×10^{-5}	9.36×10^{-5}	
		104	0.40	567.46	5.59	2.13×10^{-11}	6.12×10^{-11}	2.14×10^{-6}	8.72×10^{-6}	
		10 ⁵	0.15	out of memory						
Jacobi 2d (25 pt)	1000×1000	10 ³	0.60	4.24	0.22	1.30×10^{-7}	1.61×10^{-7}	1.35×10^{-2}	2.08×10^{-2}	
		104	0.51	out of memory						
heat 3d (7 pt)	$100 \times 100 \times 100$	10 ^{2.7}	10.35	271.52	11.81	2.21×10^{-10}	5.28×10^{-10}	2.76×10^{-5}		
		10 ³	3.31	out of me	out of memory					
Some Performance Numbers (Freespace)

_____cores: <u>48</u> (24 / socket)

SKX (Intel Skylake)

caches: 32 KB L1 / core, 1 MB L2 / core, 33 MB L3 / socket RAM: 192 GB DDR4

Stencil	Ν	Т	Running Time (sec)			Error (w.r.t. FFT)				
			Gaussian	PLuTo	FFT	Mean Squared	Max Absolute	Mean Relative	Max Relative	
heat 1d (3 pt)	$1.6 imes 10^{6}$	10 ³	0.10	0.49	0.02	1.13×10^{-12}	2.29×10^{-10}	1.20×10^{-9}	3.03×10^{-5}	
		10 ⁴	0.11	2.10	0.02	2.01×10^{-13}	2.29×10^{-11}	5.27×10^{-10}	3.03×10^{-6}	
		10 ⁵	0.11	8.73	0.02	3.58×10^{-14}	2.29×10^{-12}	2.50×10^{-10}	3.03×10^{-7}	
		10 ⁶	0.11	217.56	0.04	6.44×10^{-15}	2.30×10^{-13}	1.15×10^{-10}	3.05×10^{-8}	
		107	0.10	> 10 m	0.32	1.57×10^{-14}	5.03×10^{-14}	1.41×10^{-9}	6.74×10^{-9}	
heat 2d (5 pt)	1000×1000	10 ³	0.45	1.58	0.08	7.29×10^{-11}	3.34×10^{-10}	5.91×10^{-6}	6.36×10^{-5}	
		10 ⁴	0.42	53.74	4.55	3.12×10^{-11}	4.22×10^{-11}	3.41×10^{-6}	6.30×10^{-6}	
		10 ⁵	0.15	out of memory						
Seidel 2d (9 pt)	1000×1000	10 ³	0.40	2.41	0.08	1.23×10^{-10}	5.31×10^{-10}	1.19×10^{-5}	9.36×10^{-5}	
		10 ⁴	0.40	567.46	5.59	2.13×10^{-11}	6.12×10^{-11}	2.14×10^{-6}	8.72×10^{-6}	
		10 ⁵	0.15	out of memory						
Jacobi 2d (25 pt)	1000×1000	10 ³	0.60	4.24	0.22	1.30×10^{-7}	1.61×10^{-7}	1.35×10^{-2}	2.08×10^{-2}	
		10 ⁴	0.51	out of memory						
heat 3d (7 pt)	$100 \times 100 \times 100$	10 ^{2.7}	10.35	271.52	11.81	2.21×10^{-10}	5.28×10^{-10}	2.76×10^{-5}	1.08×10^{-4}	
		10 ³	3.31		out of memory					

Input cell values are in (0, 1]

Periodic Grids: Application of a Linear Stencil Can be Viewed as Multiplying Two Polynomials (Computing Convolution)



$$A_t(x) = v_0 + v_1 x + v_2 x^2 + v_3 x^3 + v_4 x^4 + v_5 x^5 + v_6 x^6 + v_7 x^7$$

$$a_t \quad v_0 \quad v_1 \quad v_2 \quad v_3 \quad v_4 \quad v_5 \quad v_6 \quad v_7$$

	$S_{-1}v_7$	$S_{-1}v_0$	$s_{-1}v_{1}$	$s_{-1}v_{2}$	$s_{-1}v_{3}$	$s_{-1}v_{4}$	$s_{-1}v_{5}$	$S_{-1}v_{6}$
a_{t+1}	$+ s_0 v_0$	$+ s_0 v_1$	$+ s_0 v_2$	$+ s_0 v_3$	$+ s_0 v_4$	$+ s_0 v_5$	$+ s_0 v_6$	$+ s_0 v_7$
-	$+ s_1 v_1$	$+ s_1 v_2$	$+ s_1 v_3$	$+ s_1 v_4$	$+ s_1 v_5$	$+ s_1 v_6$	$+ s_1 v_7$	$+ s_1 v_0$

$$A_{t}(x) = v_{0} + v_{1}x + v_{2}x^{2} + v_{3}x^{3} + v_{4}x^{4} + v_{5}x^{5} + v_{6}x^{6} + v_{7}x^{7}$$

$$a_{t} v_{0} v_{1} v_{2} v_{3} v_{4} v_{5} v_{6} v_{7}$$

$$s(x) = s_{1}x^{-1} + s_{0} + s_{-1}x$$
Flipped Stencil $s_{1} s_{0} s_{-1}$

$$a_{t+1} s_{0}v_{0} + s_{0}v_{1} + s_{0}v_{2} + s_{0}v_{3} + s_{0}v_{4} + s_{0}v_{5} + s_{0}v_{6} + s_{0}v_{7}$$

$$A_{t}(x) = v_{0} + v_{1}x + v_{2}x^{2} + v_{3}x^{3} + v_{4}x^{4} + v_{5}x^{5} + v_{6}x^{6} + v_{7}x^{7}$$

$$a_{t} v_{0} v_{1} v_{2} v_{3} v_{4} v_{5} v_{6} v_{7}$$

$$S(x) = s_{1}x^{7} + s_{0} + s_{-1}x \text{ (wrap around)}$$
Flipped Stencil $s_{1} s_{0} s_{-1}$

$$a_{t+1} \frac{s_{-1}v_{7}}{s_{0} s_{0} + s_{0}v_{1}}{s_{0}v_{1} + s_{0}v_{2}} \frac{s_{-1}v_{2}}{s_{0}v_{3}} \frac{s_{-1}v_{3}}{s_{0}v_{4}} \frac{s_{-1}v_{5}}{s_{0}v_{5}} \frac{s_{-1}v_{6}}{s_{0}v_{6}} \frac{s_{-1}v_{6}}{s_{0}v_{7}}$$

$$A_{t}(x) = v_{0} + v_{1}x + v_{2}x^{2} + v_{3}x^{3} + v_{4}x^{4} + v_{5}x^{5} + v_{6}x^{6} + v_{7}x^{7}$$

$$a_{t} v_{0} v_{1} v_{2} v_{3} v_{4} v_{5} v_{6} v_{7}$$

$$S(x) = s_{1}x^{7} + s_{0} + s_{-1}x \text{ (wrap around)}$$
Flipped Stencil $s_{1} s_{0} s_{-1}$

$$a_{t+1} \frac{s_{-1}v_{7}}{+s_{0}v_{0}} \frac{s_{-1}v_{0}}{+s_{0}v_{1}} \frac{s_{-1}v_{1}}{+s_{0}v_{2}} \frac{s_{-1}v_{3}}{+s_{0}v_{3}} \frac{s_{-1}v_{4}}{+s_{1}v_{5}} \frac{s_{-1}v_{5}}{+s_{0}v_{6}} \frac{s_{-1}v_{6}}{+s_{0}v_{7}}$$

$$S(x) A_{t}(x)$$

$$= (s_{0}v_{0}) + {\binom{s_{-1}v_{0}}{+s_{0}v_{1}}x} + {\binom{s_{-1}v_{1}}{+s_{0}v_{2}}x^{2}} + {\binom{s_{-1}v_{2}}{+s_{0}v_{3}}x^{3}} + {\binom{s_{-1}v_{3}}{+s_{0}v_{4}}x^{4}} + {\binom{s_{-1}v_{4}}{+s_{0}v_{5}}x^{5}} + {\binom{s_{-1}v_{5}}{+s_{0}v_{6}}x^{6}} + {\binom{s_{-1}v_{6}}{+s_{1}v_{0}}x^{7}} + {\binom{s_{-1}v_{7}}{+s_{1}v_{0}}x^{8}} + {\binom{s_{1}v_{2}}{+s_{1}v_{0}}x^{10}} + {\binom{s_{1}v_{4}}{x^{11}}} + {\binom{s_{1}v_{5}}{x^{12}}} + {\binom{s_{1}v_{6}}{x^{13}}} + {\binom{s_{1}v_{7}}{x^{14}}} + {\binom{s_{1}$$

Stencils and Polynomial Multiplication + $v_4 x^4$ $v_2 x^2$ $+ v_3 x^3$ + $v_6 x^6$ $A_t(\mathbf{x}) =$ + $+ v_5 x^5$ $+ v_7 x^7$ + $v_1 x$ v_0 a_t v_0 v_1 v_2 v_3 v_4 v_5 v_6 v_7 S(x) = $s_1 x^7$ + S_0 + $S_{-1}\boldsymbol{\chi}$ (wrap around) **Flipped** Stencil *S*₁ S_0 S_{-1} $S_{-1}v_{1}$ $S_{-1}v_{5}$ $S_{-1}v_7$ $S_{-1}v_0$ $S_{-1}v_2$ $S_{-1}v_{3}$ $S_{-1}v_4$ $S_{-1}v_{6}$ a_{t+1} $+ s_0 v_0$ $+ s_0 v_1$ $+ s_0 v_2$ $+ s_0 v_3$ $+ s_0 v_4$ $+ s_0 v_5$ $+ s_0 v_6$ $+ s_0 v_7$ $+ s_1 v_3$ $+ s_1 v_0$ $+ s_1 v_2$ $+ s_1 v_1$ $+ s_1 v_4$ $+ s_1 v_5$ $+ s_1 v_6$ $+ s_1 v_7$ $S(x) A_t(x)$ $-1v_6$ $S_{-1}v_1$ $S_{-1}v_0$ $S_{-1}v_2$ $(S_{-1}v_3)$ $\binom{S_{-1}v_5}{+s_0v_6}x^6$ $\left(S_{-1}u_{4}\right)$ x^7 $S_0 v_7$ $(s_0 v_0)$ $+s_0v_3$ $+s_0v_4$ $+s_{01}$ $+s_0v_1$ $+s_0v_2$ $S_{-1}v_7$ $+ (s_1 v_5) x^{12}$ + $(s_1 v_6) x^{13}$ (s_1v_3) (s_1v_4) $+ (s_1 v_7) x^{14}$ $(S_1 v_2)$ $+ S_1 v_1$ $s_{-1}v_{7}$ $S_{-1}v_{0}$ $(S_{-1}v_{1})$ $(s_{-1}v_{2})$ $(S_{-1}v_3)$ $(S_{-1}v_5)$ $S_{-1}v_{6}$ $(S_{-1}v_4)$ $r^2 +$ $+s_0v_3$ $x^{3} + +s_{0}v_{4} x^{4} +$ $+s_0v_5 x^5 +$ $+s_0v_6 x^6 +$ $x + + s_0 v_2$ $+s_0v_0$ + $+s_0v_1$ $+s_0v_7$ χ^7 $+S_1v_3$ $+s_1v_5$ $+s_1v_6$ $+S_1v_1$ $+S_1v_2$ $+S_1 v_4$ $+s_1v_7$ $+s_1v_0$

 $=A_{t+1}(x)$



This can be computed using repeated squaring ($O(\log T)$ polynomial products)

Computational complexity of multiplying two polynomials of degree bound N:

Classical Algorithm: $\Theta(N^2)$ Karatsuba's Algorithm: $\Theta(N^{\log_2 3}) \in O(N^{1.59})$ Toom-Cook Algorithms

Fast Fourier Transform (FFT): $\Theta(N \log N)$



Stencil S



Initial data a_0









Computational Complexity: $\Theta(N \log(NT))$ (for a *d*-dimensional $N^{\frac{1}{d}} \times N^{\frac{1}{d}} \times \cdots \times N^{\frac{1}{d}}$ grid with constant *d*) Aperiodic Grids: Aperiodic Algorithm is a Repeated Application of Periodic Algorithm via Divide-and-Conquer

The region of influence of a grid point p consists of the set of grid points whose values can depend on the value at point p.



region of influence (entire green region)

The region of influence of a grid point p consists of the set of grid points whose values can depend on the value at point p.



region of influence (entire green region)























encountered before!











encountered before!










encountered before!





encountered before!











encountered before!











Computational Complexity:

$$\Theta\left(TN^{1-\frac{1}{d}}\log(TN^{1-\frac{1}{d}})\log T + N\log N\right)$$

(for a *d*-dimensional $N^{\frac{1}{d}} \times N^{\frac{1}{d}} \times \cdots \times N^{\frac{1}{d}}$ grid with constant *d*

How Good is the Aperiodic Algorithm?

Computational Complexity for a *d*-dimensional hypercubic $\left(N^{\frac{1}{d}} \times N^{\frac{1}{d}} \times \cdots \times N^{\frac{1}{d}}\right)$ grid (assuming constant *d*):

 $\Theta\left(TN^{1-\frac{1}{d}}\log\left(TN^{1-\frac{1}{d}}\right)\log T + N\log N\right)$

Т

 $N\frac{1}{2}$

 $N^{\frac{1}{2}}$

But when T timesteps are executed on such a grid, the number of cells on the boundary is $2d TN^{1-\frac{1}{d}} = \Theta(TN^{1-\frac{1}{d}})$.

If the boundary cells can take arbitrary values, one must read every boundary cell for correctness.

Thus, one is forced to do $\Omega(TN^{1-\frac{1}{d}})$ work in such a case.

Hence, for large T and arbitrary boundary conditions, the aperiodic algorithm is within polylog factor of optimal.

Freespace Grids: Freespace has a Space Problem

Freespace May Blow up Space (and Time)





Freespace May Blow up Space (and Time)



Freespace May Blow up Space (and Time)



for *d*-dimensional hypercubic $\left(N^{\frac{1}{d}} \times N^{\frac{1}{d}} \times \cdots \times N^{\frac{1}{d}}\right)$ grids with constant *d*

Freespace Grids: S^{∞} is a Gaussian S^T Approximates a Gaussian

Normalized Nonnegative Stencils

We assume that Stencil S is

- linear,
- composed of nonnegative weights only, and
- normalized so that all weights add up to 1.









after various timesteps

walker location probabilities after various number of steps









0.2

0.4

0.4

probabilities:





grid cell values after various timesteps



walker location probabilities after various number of steps





step



walker location probabilities after various number of steps









walker location probabilities after various number of steps



Normalized Nonnegative Stencils and Tracking a Bunch of Drunk Walkers





expected #walkers in each cell after 3 steps



expected #walkers in each cell after various number of steps



Normalized Nonnegative Stencils and Tracking a Bunch of Drunk Walkers





expected #walkers in each cell after 3 steps



expected #walkers in each cell after various number of steps
























Grid Index

random walk



Grid Index







Grid Index

random walk















S^T Approximates a Gaussian A linear stencil with nonnegative weights can be modeled as a random walk on an integer grid.

Given a *d*-dimensional stencil *S* we can compute the mean vector μ_T and covariance matrix Σ_T of S^T in O(1) time.

Then S^T approximates the following Gaussian:

$$G_{\mu_T, \Sigma_{\rm T}}(x) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma_{\rm T})}} e^{-\frac{1}{2}(x-\mu_T)^{trans} \Sigma_{\rm T}^{-1}(x-\mu_T)}$$

Let *S* be a <u>linear stencil</u> with

expectation 0 (symmetric)

variance σ^2

skewness ρ

Let $G_{T\sigma^2}(x)$ be a <u>Gaussian</u> with expectation 0 variance $T\sigma^2$

Then for any integer \boldsymbol{x} :

$$\left|S^{T}[x] - G_{T\sigma^{2}}(x)\right| \leq \frac{1}{\sigma\sqrt{T}} \left(\frac{2C\rho}{\sigma} + \frac{1}{\sqrt{2\pi e}}\right)$$

where, $C \le 0.4748$.

Algorithm for Freespace Grids







This is a very structured version of the *n*-body problem with a Gaussian interaction function!

So, we can use a fast multipole type algorithm to find an approximate solution efficiently.

The algorithm works by approximating the Gaussian S^{T} approximates!

Algorithm for Freespace Grids



Computational Complexity: $\Theta\left(N\log^{O(d)}\left(\frac{1}{\epsilon}\right) + \log T\right)$ (for a *d*-dimensional $N^{\frac{1}{d}} \times N^{\frac{1}{d}} \times \cdots \times N^{\frac{1}{d}}$ grid with constant *d*)

How About Nonlinear Stencils?

Binomial and Black-Scholes-Merton Option Pricing (American Options)

- Modeled as an aperiodic nonlinear 1D stencil computation problem with a max operator
- Requires $O(N^2)$ work using standard algorithms, where N =#timesteps (= grid size)
- Can be reduced into linear 1D stencil computation problems through recursive decomposition
- The FFT-based periodic linear stencil algorithm for 1D grids \Rightarrow the nonlinear American option pricing problem can be solved in $O(N \log^2 N)$ work

Stencil Weights are Functions of Space and/or Time Coordinates

- Some of these problems can be reduced to a sequence of linear stencil computation problems
- Inside each linear stencil computation phase, we use fixed approximate stencil weights based on the actual space/time-dependent weights of the original stencil
- The final output approximates the final grid values

Some Open Problems

- Efficient algorithms for classes of nonlinear stencils.
- Low-span algorithms for aperiodic stencils.
- Algorithms for inhomogenous stencils.
- Stencil code generator that combines trapezoidal decomposition, tiling, FFT, Gaussians, etc. to achieve the best performance under a given set of constraints (e.g., error tolerance, space bound).
 We already have FOURST — a very primitive FFT
 - based generator.

GITHUB Repository for FFT-based Stencil Codes

https://github.com/TEAlab/FFTStencils