Cache Oblivious Stencil Computations

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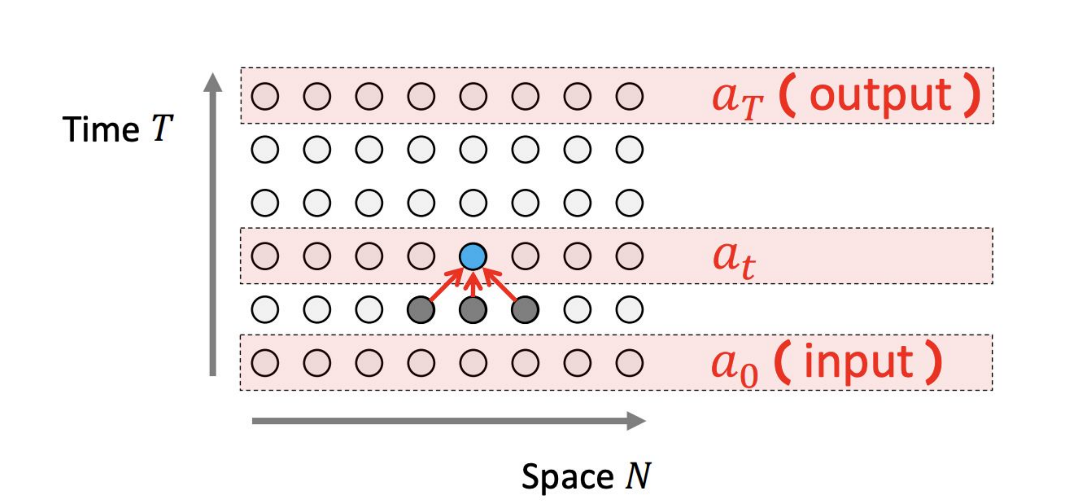
Stencil Computations

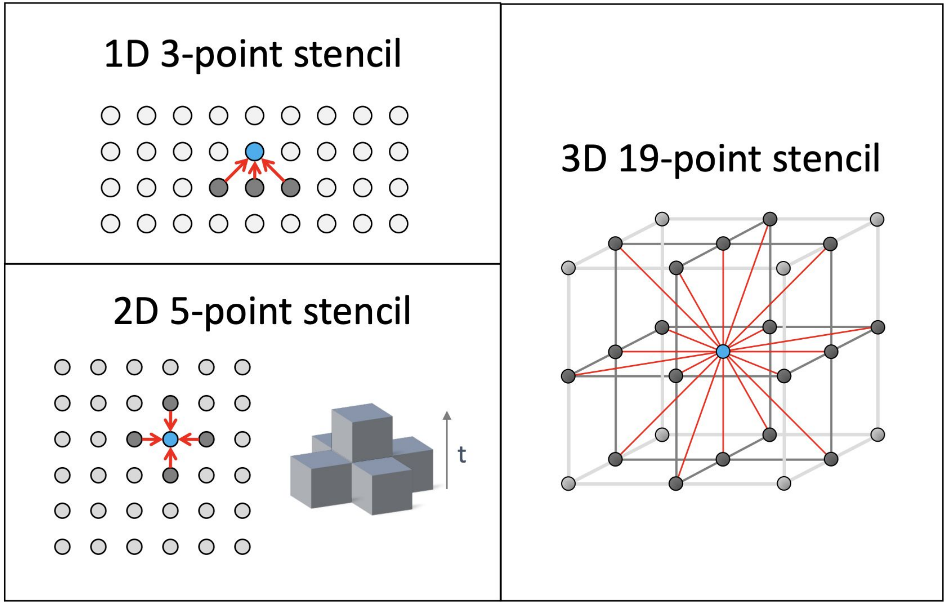
what is a stencil?

- a computation defined on an n dimensional grid along with a time parameter t
- each value on the grid at a time t is a function of the neighboring grid cells at time t-1, t-2, …, t-k
- the input is a set of initial value a0 while the output T time steps later is aT



examples

- if a stencil is a p-point stencil, the value depends on its p neighbors in the previous timestep.
- the n dimensions plus the time dimension together span the (n+1) dimension spacetime.



heat diffusion

- one notable example is heat diffusion which represents a 5-point 2D stencil on a discrete grid:
- the update function is known as the computational kernel

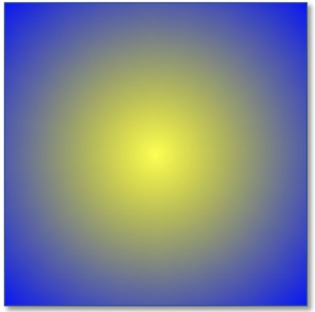
Let $h_t(x, y)$ be the heat at point (x, y) at time t.

Heat Equation

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

Update Equation (on a discrete grid)

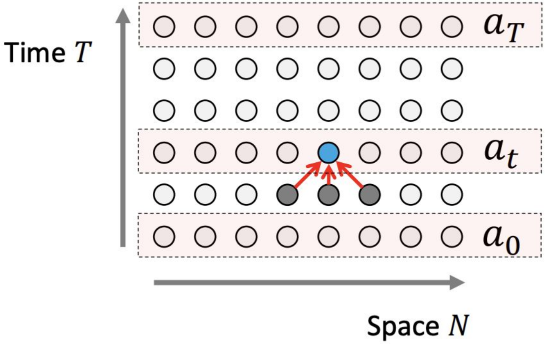
$$h_{t+1}(x, y) = h_t(x, y)$$
$$+c_x\big(h_t(x+1, y) - 2h_t(x, y) + h_t(x-1, y)\big)$$
$$+c_y\big(h_t(x, y+1) - 2h_t(x, y) + h_t(x, y-1)\big)$$



Stencil Computation Algorithms

standard implementation

- the naive algorithm involves applying the computational kernel to all points at time step t before timestep t+1
- If the number of points in at each time step exceeds the cache size Z, this computation incurs O(p) cache misses where p is the number of points computed



for $t \leftarrow 1$ to T **do**
  for $i \leftarrow 0$ to $N-1$ **do**
    compute $a_t[i]$ from a_{t-1}
    using the stencil

main result

- The paper presents a novel stencil computation algorithm that when traversing a large rectangular region of (n+1) dimensional spacetime, incurs $O(p/Z^{n+1})$ cache misses.
    - this matches a lower bound proved by Hong and Kong [3] by a constant factor
    - applies to arbitrary stencil and dimension
- this algorithm is also cache oblivious
    - does not contain the cache size as a parameter

One-Dimensional Stencil Algorithm

walk1

- we define a procedure walk1 that traverses a rectangular region 0 <= t < T and 0 <= x < N
- for simplicity, we restrict the computation to a 3 point stencil
  - (t, x) depends on (t-1, x-1), (t-1, x), (t-1, x+1)
- instead of just considering rectangular regions, we instead consider a more general trapezoidal region with additional parameters x0 and x1 dot.

```
void walk1(int t0, int t1, int x0, int ẋ0, int x1, int ẋ1)
{
    int Δt = t1 - t0;

    if (Δt == 1) {
        /* base case */
        int x;
        for (x = x0; x < x1; ++x)
            kernel(t0, x);
    } else if (Δt > 1) {
        if (2 * (x1 - x0) + (ẋ1 - ẋ0) * Δt >= 4 * Δt) {
            /* space cut */
            int xm = (2 * (x0 + x1) + (2 + ẋ0 + ẋ1) * Δt) / 4;
            walk1(t0, t1, x0, ẋ0, xm, -1);
            walk1(t0, t1, xm, -1, x1, ẋ1);
        } else {
            /* time cut */
            int s = Δt / 2;
            walk1(t0, t0 + s, x0, ẋ0, x1, ẋ1);
            walk1(t0 + s, t1, x0 + ẋ0 * s, ẋ0, x1 + ẋ1 * s, ẋ1);
        }
    }
}
```

trapezoid

For integers $t_0, t_1, x_0, \dot{x}_0, x_1, \dot{x}_1$ we define trapezoid $\mathcal{T}(t_0, t_1, x_0, \dot{x}_0, x_1, \dot{x}_1)$ to be the set of points that satisfy $t_0 \le t < t_1,\ x0 + \dot{x}_0(t - t_0) \le x < x_1 + \dot{x}_1(t - t_0)$.

The height is computed as $\Delta T = t_1 - t_0$

The width is the average lengths of the parallel sides: $w = (x_1 - x_0) + (\dot{x}_1 - \dot{x}_0)\Delta T/2$

The center is the average of the four corners:

$x = (x_0 + x_1)/2 + (\dot{x}_0 + \dot{x}_1)\Delta t/4$

The volume |T| is the number of points in the trapezoid.

Assume for now that the special case with slopes zero denotes the rectangular region.

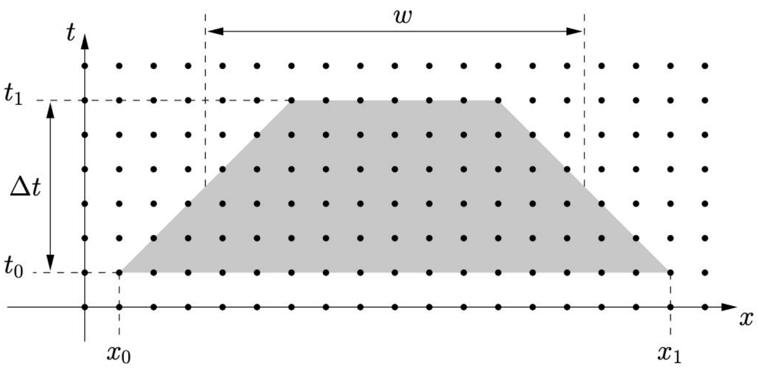


Figure 2: Illustration of the trapezoid $\mathcal{T}(t_0, t_1, x_0, \dot{x}_0, x_1, \dot{x}_1)$ for $\dot{x}_0 = 1$ and $\dot{x}_1 = -1$. The trapezoid includes all points in the shaded region, except for those on the top and right edges.

walk1 steps

- the algorithm works by recursively decomposing the region into smaller rectangles
- The base case is when the height is one
- Otherwise we perform one of two cuts dividing the trapezoid in half, recursing on each one

Base case: If the height is 1, then the trapezoid consists of the line of spacetime points (t_0, x) with $x_0 \leq x < x_1$. The procedure visits all these points, calling the application-specific procedure **kernel**. The traversal order is not important because these points do not depend on each other.

```
int Δt = t1 - t0;

if (Δt == 1) {
    /* base case */
    int x;
    for (x = x0; x < x1; ++x)
        kernel(t0, x);
```

Space Cut

- If the width is long enough, perform a diagonal cut from the center splitting the region into another trapezoid and a parallelogram. Then recurse on the trapezoid first.

Space cut: If the width is at least twice the height, then we cut the trapezoid along the line with slope -1 through the center of the trapezoid, cf. Fig. 3. The recursion first traverses trapezoid $\mathcal{T}_1 = \mathcal{T}(t_0, t_1, x_0, \dot{x}_0, x_m, -1)$, and then trapezoid $\mathcal{T}_2 = \mathcal{T}(t_0, t_1, x_m, -1, x_1, \dot{x}_1)$. This traversal order is valid because no point in $\mathcal{T}_1$ depends upon any point in $\mathcal{T}_2$.

From Fig. 3, we obtain

$$x_m = \frac{1}{2}(x_0 + x_1) + \frac{1}{4}(\dot{x}_0 + \dot{x}_1)\Delta t + \frac{1}{2}\Delta t \ .$$

```
if (2 * (x_1 - x_0) + (ẋ_1 - ẋ_0) * Δt >= 4 * Δt) {
    /* space cut */
    int x_m = (2 * (x_0 + x_1) + (2 + ẋ_0 + ẋ_1) * Δt) / 4;
    walk1(t_0, t_1, x_0, ẋ_0, x_m, -1);
    walk1(t_0, t_1, x_m, -1, x_1, ẋ_1);
```

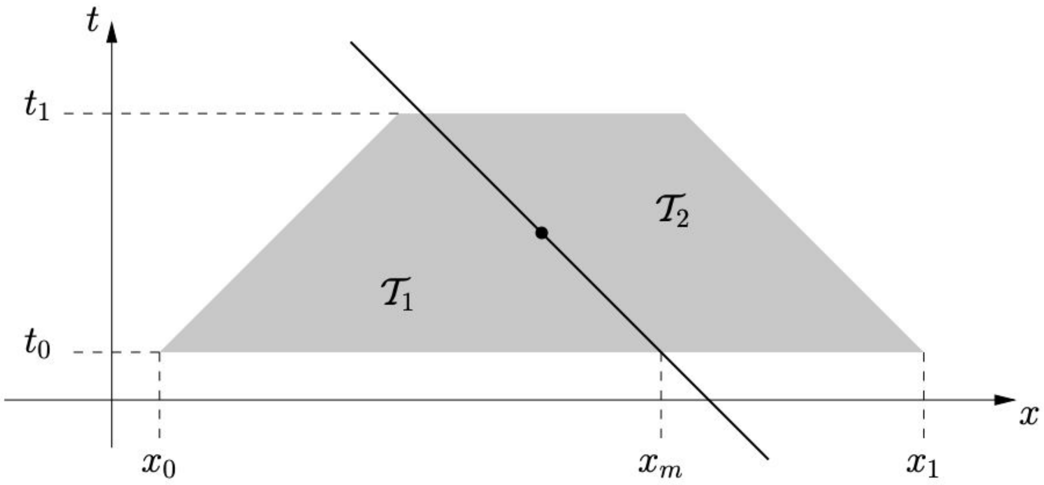


Figure 3: Illustration of a *space cut*. When the space dimension is "large enough" (see text), procedure `walk1` cuts the trapezoid along the line of slope -1 through its center.

time cut

- otherwise perform a timecut dividing the region into two trapezoids by cutting horizontally through the center. Then recurse on the bottom region first

Time cut: Otherwise, we cut the trapezoid along the horizontal line through the center, cf. Fig. 4. The recursion first traverses trapezoid $\mathcal{T}_1 = \mathcal{T}(t_0, t_0 + s, x_0, \dot{x}_0, x_1, \dot{x}_1)$, and then trapezoid $\mathcal{T}_2 = \mathcal{T}(t_0 + s, t_1, x_0 + \dot{x}_0 s, \dot{x}_0, x_1 + \dot{x}_1 s, \dot{x}_1)$, where $s = \Delta t/2$. The order of these traversals is valid because no point in $\mathcal{T}_1$ depends on any point in $\mathcal{T}_2$.

```
} else {
    /* time cut */
    int s = Δt / 2;
    walk1(t0, t0 + s, x0, ẋ0, x1, ẋ1);
    walk1(t0 + s, t1, x0 + ẋ0 * s, ẋ0, x1 + ẋ1 * s, ẋ1);
}
```

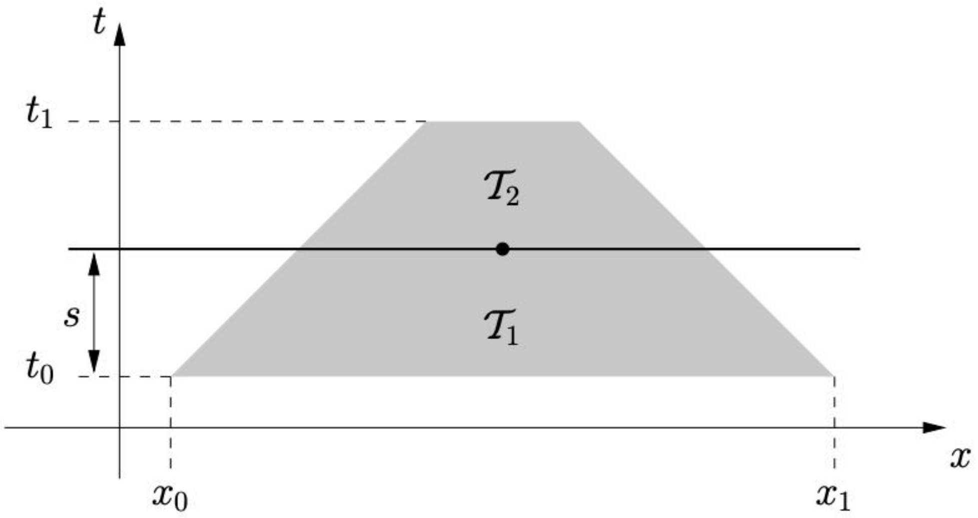
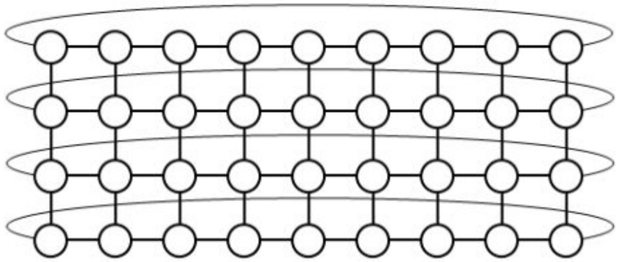
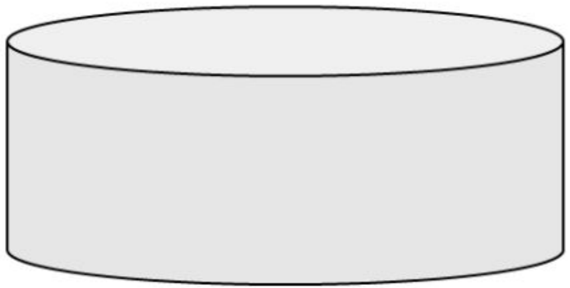


Figure 4: Illustration of a *time cut*: procedure `walk1` cuts the trapezoid along the horizontal line through its center.

summary

- we can guarantee that both cuts always produce valid and well defined regions.
- we can show that this procedure also works on cylindrical where (t+1, x) depends on (t, (x-1) mod N), (t, x mod N), (t, (x+1) mod N).





cylindrical traversal

- traversal order for cylindrical traversal where N=T=10

$t \backslash x$	0	1	2	3	4	5	6	7	8	9
9	79	88	89	90	94	95	97	98	99	78
8	76	77	85	86	87	92	93	96	74	75
7	71	72	73	82	83	84	91	68	69	70
6	62	63	66	67	80	81	54	55	58	59
5	57	60	61	64	65	50	51	52	53	56
4	45	47	48	49	28	29	38	39	40	44
3	42	43	46	24	25	26	27	35	36	37
2	34	41	18	19	20	21	22	23	32	33
1	31	4	5	8	9	12	13	16	17	30
0	0	1	2	3	6	7	10	11	14	15

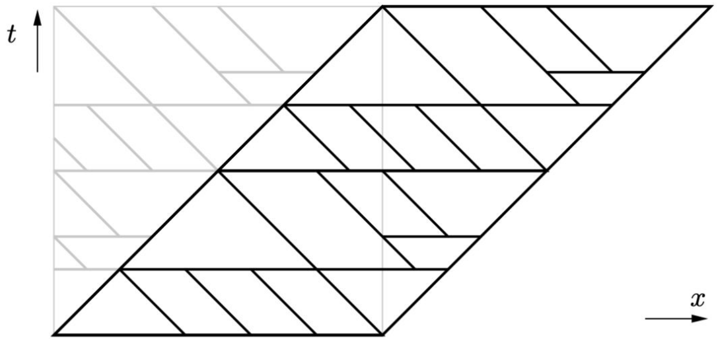


Figure 5: Cache-oblivious traversal of 1-dimensional spacetime for $N = T = 10$.

Extension to Multiple Dimensions and Arbitrary Stencils

arbitrary stencils

- we first extend walk1 to a spacetime point (t+1, x) to depend on any (t, x+k) for any $|x-k| \leq \sigma^2$
- To do this, we simply modify our space cut so that we cut along the center with a line of slope $dx/dt = -\sigma$. This guarantees that two point in the first region depends on a point in the second region. This cut can be applied whenever $w \geq 2\sigma\Delta t,$ which guarantees the two regions are well defined.

arbitrary dimension

- We extend the definition of the 2D trapezoid to an arbitrary number of dimensions
- If any of the dimensions permits a space cut, we cut along that dimension and recurse, otherwise we perform a time cut
- As the projection onto any dimension matches our 2D case, this algorithm also generates a valid stencil traversal.

A n-dimensional trapezoid $\mathcal{T}(t_0, t_1, x_0^{(i)}, \dot{x}_0^{(i)}, x_1^{(i)}, \dot{x}_1^{(i)})$, where $0 \leq i < n$, is the set of integer tuples $(t, x^{(0)}, x^{(1)}, \ldots, x^{(n-1)})$ such that $t_0 \leq t < t_1$ and $x_0^{(i)} + \dot{x}_0^{(i)}(t - t_0) \leq x^{(i)} < x_1^{(i)} + \dot{x}_1^{(i)}(t - t_0)$ for all $0 \leq i < n$. Informally, for each dimension i, the projection of the multi-dimensional trapezoid onto the $(t, x^{(i)})$ plane looks like the 1-dimensional trapezoid in Fig. 2.

```
typedef struct { int x₀, ẋ₀, x₁, ẋ₁ } C;

void walk(int t₀, int t₁, C c[n])
{
    int Δt = t₁ - t₀;

    if (Δt == 1) {
        basecase(t₀, c);
    } else if (Δt > 1) {
        C *p;

        /* for all dimensions, try to cut space */
        for (p = c; p < c + n; ++p) {
            int x₀ = p->x₀, x₁ = p->x₁, ẋ₀ = p->ẋ₀, ẋ₁ = p->ẋ₁;
            if (2 * (x₁ - x₀) + (ẋ₁ - ẋ₀) * Δt >= 4 * σ * Δt) {
                /* cut space dimension *p */
                C save = *p;   /* save configuration *p */
                int xₘ = (2 * (x₀ + x₁) + (2 * σ + ẋ₀ + ẋ₁) * Δt) / 4;
                *p = (C){ x₀, ẋ₀, xₘ, -σ };   walk(t₀, t₁, c);
                *p = (C){ xₘ, -σ, x₁, ẋ₁ };   walk(t₀, t₁, c);
                *p = save;     /* restore configuration *p */
                return;
            }
        }

        {
            /* because no space cut is possible, cut time */
            int s = Δt / 2;
            C newc[n];
            int i;

            walk(t₀, t₀ + s, c);

            for (i = 0; i < n; ++i) {
                newc[i] = (C){ c[i].x₀ + c[i].ẋ₀ * s, c[i].ẋ₀,
                               c[i].x₁ + c[i].ẋ₁ * s, c[i].ẋ₁ };
            }

            walk(t₀ + s, t₁, newc);
        }
    }
}
```

Cache Analysis

Theorem

- We will prove that the walk algorithm incurs $O(\mathrm{Vol}(\mathcal{T})/Z^{1/n})$ caches misses under certain assumptions
  - the kernel operates in place meaning $(t, x^{(0)}, x^{(1)}, \ldots, x^{(n-1)})$ is stored in the same memory locations as $(t-k, x^{(0)}, x^{(1)}, \ldots, x^{(n-1)})$.
  - the cache is ideal (optimal replacement policy) and fully associative
  - the trapezoid is “sufficiently large”

Lemma 1

Lemma 1 Let $\mathcal{T}$ be the n-dimensional trapezoid $\mathcal{T}(t_0, t_1, x_0^{(i)}, \dot{x}_0^{(i)}, x_1^{(i)}, \dot{x}_1^{(i)})$, where $0 \leq i < n$. Let $\mathcal{T}$ be well-defined, w_i be the width of the trapezoid in dimension i, and let $m = \min(\Delta t, w_0, w_1, \ldots, w_{n-1})/2$. Then, there are $O((1+n)\mathrm{Vol}(\mathcal{T})/m)$ points on the surface of the trapezoid.

Proof: The volume of the trapezoid is the sum for all time slices of the number of points in the (rectangular) slice:

$$\mathrm{Vol}(\mathcal{T}) = \sum_{-\Delta t/2 \leq t < \Delta t/2} \prod_{0 \leq i < n} (w_i + \vartheta_i t) \ ,$$

where $\vartheta_i = \dot{x}_1^{(i)} - \dot{x}_0^{(i)}$. Define the auxiliary function

Lemma 1

- Define the auxiliary function which represents the volume of the spacetime region with an additional +/- s. The surface area is then V(1) - V(0)

$$V(s) = \sum_{-(\Delta t/2)-s \leq t < (\Delta t/2)+s} \prod_{0 \leq i < n} (w_i + 2s + \vartheta_i t) .$$

- This value is upper bounded by the integral

$$V(s) = \int_{-(\Delta t/2)-s}^{(\Delta t/2)+s} \prod_{0 \leq i < n} (w_i + 2s + \vartheta_i t) \, dt$$

Lemma 1

- After the substitution $t = (m+s)r$, we obtain

$$V(s) = \int_{-g(s)}^{g(s)} (m+s) f(s,r)\, dr \ ,$$

where $g(s) = ((\Delta t/2) + s)/(m+s)$ and

$$f(s,r) = \prod_{0 \le i < n} (w_i + (2 + \vartheta_i r)s + \vartheta_i rm)$$

The derivative $V'(0)$ is

$$V'(0) = g'(0) \cdot m \cdot \big(f(0, g(0)) + f(0, -g(0))\big) + \int_{-g(0)}^{g(0)} \left(f(0,r) + m \cdot \left. \frac{df(s,r)}{ds} \right|_{s=0} \right) dr \ . \tag{2}$$

Observe that

$$m \cdot \left. \frac{df(s,r)}{ds} \right|_{s=0} = f(0,r) \cdot \sum_{0 \le j < n} \frac{2m + \vartheta_j rm}{w_j + \vartheta_j rm} \le n f(0,r) \ , \tag{3}$$

where the inequality holds because $(2m + \vartheta_j rm)/(w_j + \vartheta_j rm) \le 1$, which holds because we have $2m \le w_j$ by definition of m, and because we have $w_j + \vartheta_j rm \ge 0$ since the trapezoid is well-defined.

Further observe that, because $m \le \Delta t/2$ holds by definition of m, we have that $g'(s) = (m - \Delta t/2)/(m+s)^2 \le 0$. Because the trapezoid is well-defined, we have $f(s,r) \ge 0$ and $m \ge 0$. Therefore, we obtain

$$g'(0) \cdot m \cdot \big(f(0, g(0)) + f(0, -g(0))\big) \le 0 \ . \tag{4}$$

By substituting Eqs. (3) and (4) into Eq. (2), we obtain the result $V'(0) \le (1+n)V(0)/m$, and the lemma follows. Q.E.D.

Main Theorem

Theorem 2 Let $\mathcal{T}$ be the well-defined n-dimensional trapezoid $\mathcal{T}(t_0, t_1, x_0^{(i)}, \dot{x}_0^{(i)}, x_1^{(i)}, \dot{x}_1^{(i)})$. Let procedure `walk` traverse $\mathcal{T}$ and execute a kernel in-place on a machine with an ideal cache of size Z. Assume that $\Delta t = \Omega(Z^{1/n})$ and that $w_i = \Omega(Z^{1/n})$ for all i, where w_i is the width of the trapezoid in dimension i. Then, procedure `walk` incurs at most $O(\mathrm{Vol}(\mathcal{T})/Z^{1/n})$ cache misses.

- We recursively divide the trapezoid into smaller trapezoids until we reach a sub-trapezoid S with O(Z) surface points. Due to the in-place memory assumption, we can compute the points in S with $O(\partial\mathrm{Vol}(\mathcal{S}))$ e misses (replaces happen in cache)
- For S, we know $\Delta t = \Theta(w_i)$ since otherwise, the corresponding dimension would be cut. Therefore, $\Delta t = \Omega((\partial\mathrm{Vol}(\mathcal{S}))^{1/n}) = \Omega(Z^{1/n})$.
- From Lemma 1, $\partial\mathrm{Vol}(\mathcal{S}) = O(\mathrm{Vol}(\mathcal{S})/\Delta t)$. from which it follows that the number of cache misses from computing S is $O(\mathrm{Vol}(\mathcal{S})/Z^{1/n})$. Summing over all S, we arrive at the result.

Conclusion

- Future Work
  - Conduct an empirical analysis with real hardware to compare practical cache miss rate
  - Consider cache complexity for multithreaded/parallel versions of walk
- Strengths
  - Algorithm is broadly applicable as its the first of its time to generalize to arbitrary stencils and dimensions
  - Bound reaches theoretical limit
- Weaknesses
  - Needs more empirical testing along with real hardware
  - Makes significant assumptions on the structure of the stencil and types of cache