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Numerical Solution of Laplace’s Equation

Implementing a high performance solver and conducting performance analysis

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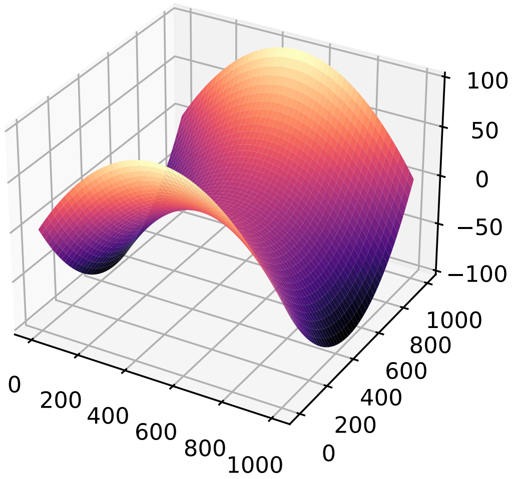
The Laplace equation



$$f : \mathbb{R}^n \to \mathbb{R}$$

$$\Delta f = 0$$

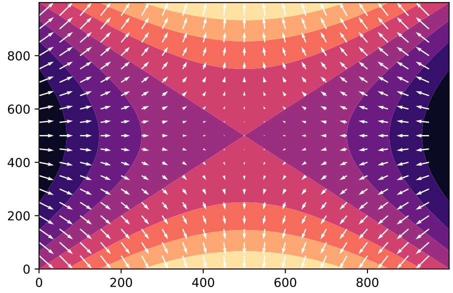
$$\Delta f = \nabla^2 f = \text{div grad } f$$

$$\nabla = \left(\frac{\partial}{\partial x_1}, \dots \frac{\partial}{\partial x_n}\right)$$

left: $f(x, y) \approx x^2 - y^2$

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 2 - 2 = 0\checkmark$$

Laplace Operator



$\nabla f = \text{grad } f = \left(\frac{\partial f}{\partial x_1}, \ldots \frac{\partial f}{\partial x_n}\right) =$ first order derivative of f

$\nabla^2 f = \frac{\partial^2 f}{\partial x_1^2} + \ldots + \frac{\partial^2 f}{\partial x_n^2} =$ second order derivative of f

Intuition

$\Delta f = 0$

- No max or min
- In 2D: $\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0 \rightarrow \frac{\partial^2 f}{\partial x^2} = -\frac{\partial^2 f}{\partial y^2}$
  - Curvature in one dimension cancels curvature in other direction
- Equilibrium equation
- Influx equals efflux at every point

Applications

Gauß’s law for **gravity**:Gauß’s law for **gravity**:

$$\nabla g = -4\pi G\rho$$

$$g = -\nabla\phi$$

Poisson’s equation for gravitational fields:

$$\Delta\phi = 4\pi G\rho$$

$$\rho = 0 \rightarrow \Delta\phi = 0$$

Laplace’s equation for

Heat equation:

$$\frac{\partial}{\partial t}u(x,t) = -a\Delta_x u(x,t)$$

$\frac{\partial}{\partial t}u(x,t) = 0 \rightarrow$ Laplace equation

Electrostatics:

$$\mathbf{E} = -\nabla V_{\mathbf{E}}$$

$$\nabla\mathbf{E} = \nabla(-\nabla V_{\mathbf{E}})$$

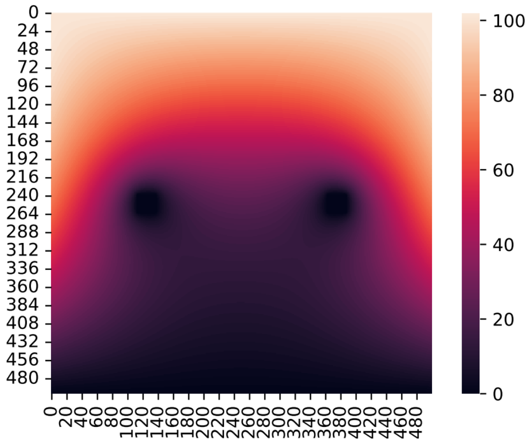
$$= -\Delta V_{\mathbf{E}} = \rho\varepsilon_0$$

$V_{\mathbf{E}}$ satisfies Laplace equation where $\rho = 0$

Boundary Conditions

- Laplace equation
  - infinitely many solutions
- Dirichlet boundary conditions
  - fixed continuous values at some boundary
- Dirichlet boundary conditions
  - unique solution

Solutions



Analytic solution infeasible

Goal

- We created numeric solver
- Scales to large problem size on a cluster

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Finite element method

Discretize domain into grid cells with spacing *h*:

$$u_{i,j+1} = f(x, y+h)$$

$$u_{i-1,j} = f(x-h, y) \qquad u_{i,j} = f(x, y) \qquad u_{i+1,j} = f(x+h, y)$$

$$u_{i,j-1} = f(x, y-h)$$

Finite difference method

Approximate Laplace operator at grid cells.
By Taylor expansion in x-dimension:

$$u_{i+1,j} \approx u_{i,j} + h\frac{\partial f}{\partial x} + \frac{1}{2}h^2\frac{\partial^2 f}{\partial x^2}$$

$$u_{i-1,j} \approx u_{i,j} - h\frac{\partial f}{\partial x} + \frac{1}{2}h^2\frac{\partial^2 f}{\partial x^2}$$

Then:

$$u_{i+1,j} + u_{i-1,j} \approx 2u_{i,j} + h^2\frac{\partial^2 f}{\partial x^2}$$

Finite difference method

Similarly for y-dimension:

$$u_{i,j+1} + u_{i,j-1} \approx 2u_{i,j} + h^2 \frac{\partial^2 f}{\partial y^2}$$

Adding both together leads to:

$$\Delta f \approx (u_{i,j+1} + u_{i,j-1} + u_{i+1,j} + u_{i-1,j} - 4u_{i,j})/h^2$$

Since $\Delta f = 0$:

$$u_{i,j} \approx (u_{i,j+1} + u_{i,j-1} + u_{i+1,j} + u_{i-1,j})/4$$

Each grid cell is roughly the average of its neighbors!

Relaxation

- $n \times n$ grid
  - n^2 linear equations
  - Solving directly infeasible
- **Relaxation** method
  - Iteratively apply approximation to grid cells until convergence
    - Jacobi: out-of-place, pleasingly parallel
    - Gauß-Seidel: in-place, twice as fast, sequential, allows overrelaxation
  - $\mathcal{O}(n^2)$ iterations, $\mathcal{O}(n^4)$ runtime.

Overrelaxation

Idea: overcorrecting with $w \in [1, 2)$

$$\text{next} = u + w * (\text{average} - u)$$

$\mathcal{O}(n)$ iterations, $\mathcal{O}(n^3)$ runtime.

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- Functions
- Problems with Sequential

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Function: data struct

```
struct Data {
    std::ptrdiff_t width;
    std::ptrdiff_t height;
    std::vector<scalar_t> data;

    scalar_t& idx(std::ptrdiff_t x, std::ptrdiff_t y) {
        return data[x + width * y];
    }
};
```

Function: get_input 1

```
Data get_input() {
    const int heat = 100;

    Data input;
    input.width = 1000;
    input.height = 1000;
    input.data.resize(input.width*input.height, std::numeric_limits<scalar_t
    ↪ >::quiet_NaN());
    //see next slide
}
```

Function: get_input 2

```cpp
for (auto y = 0z; y < input.height; ++y) {
    for (auto x = 0z; x < input.width; ++x) {
        if (y == 0) {
            input.idx(x,y) = heat;
        } else if (x == 0 || x == input.width-1 || y == input.height-1) {
            input.idx(x,y) = 0;
        }
    }
}

return input;
```

Function: get_variable_coordinates

```cpp
std::vector<Coordinate> variable_coordinates;

for (auto y = 0z; y < data.height; ++y) {
    for (auto x = 0z; x < data.width; ++x) {
        if (std::isnan(data.idx(x,y))) {
            if (is_border(x,y)) {
                throw std::runtime_error{"Error"};
            }
            variable_coordinates.push_back({x,y});
        }
    }
}
return variable_coordinates;
```

Function: make_first_guess

```cpp
void make_first_guess(Data& data, const std::vector<Coordinate>&
    ↪ variable_coordinates) {
    for (auto [x, y] : variable_coordinates) {
        data.idx(x,y) = 0;
    }
}
```

Function: zeitschritt

```
const auto max_iterations = 10000;
    auto i = 0;
    for (; i < max_iterations; ++i) {
        scalar_t residual = 0;
        for (auto [x,y] : variable_coordinates) {
            const auto old_value = data.idx(x,y);
            const auto average = (data.idx(x,y-1) + data.idx(x-1,y) + data.idx
    ↪ (x+1,y) + data.idx(x,y+1)) / 4;
            data.idx(x,y) = data.idx(x,y) + relaxation_factor * (average -
    ↪ data.idx(x,y));
            residual += std::pow(data.idx(x,y) - old_value, 2);
        }
        if (residual < precision) {
            break;
        }
    }
```

Problems with sequential version

- Higher accuracy $\rightarrow$ Bigger Grid
  - Needs more Performance
- Bigger Grid $\rightarrow$ More iterations to converge
  - Also needs more Performance

$\Rightarrow$ Parallelization needed!

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- Parallelization Approach
- Parallelization Difficulties

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Parallelization approach

- Split up iterations or grid
  - Iterations can’t be split
    - Every iteration depends on previous one

Parallelization approach

- Split up iterations or grid
  - Iterations can't be split
    - Every iteration depends on previous one
- Grid needs to be split!
  - Means that boundarys have to be communicated

Parallelization difficulties

- Find a way to split the grid

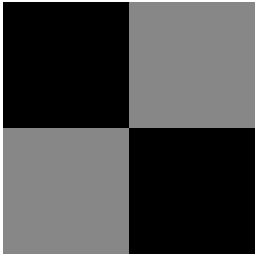
Figure: Split in 2 dimensions

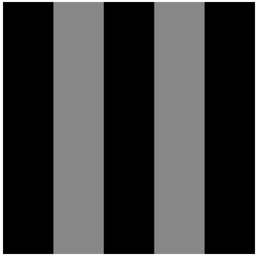
Figure: Split in 1 dimension

Parallelization difficulties

- Find a way to split the grid

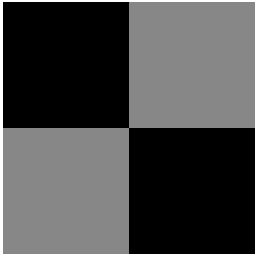

Figure: Split in 2 dimensions

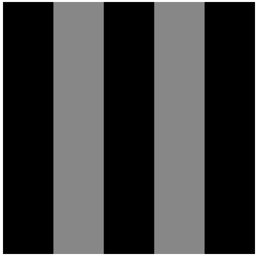

Figure: Split in 1 dimension

- one dimension is easier to initialize!

Divide the grid

```
auto smaller_tasks_size = input.global_width / world.size();
auto smaller_task_amount = world.size() - input.global_width % world.size();

if(world.rank() < smaller_task_amount){
    input.width = lower_local_width
}
else{
    input.width = lower_local_width + 1
}

input.height = size;
```

Function: get_input

- Uses data from grid division

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- Every thread gets it’s local borders...

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- ...and storage space for it’s and it’s neighbours data

Function: get_input

- Uses data from grid division
- Every thread gets it’s local borders...
- ...and storage space for it’s and it’s neighbours data
- Otherwise works as in the sequential

Parallelization difficulties

- Communicating the borders
  - After every iteration
  - Using sendrecieve

```
if (const auto result = MPI_Sendrecv(
      &data.idx(0, 0), data.height, mpi_type_scalar, left_neighbor, 0,
      &data.idx(data.width, 0), data.height, mpi_type_scalar,
      right_neighbor, 0, cart, MPI_STATUS_IGNORE
);

result != MPI_SUCCESS) {
throw mpi::exception{"MPI_Sendrecv", result};
}
```

Parallelization difficulties

- Residual needs to be communicated
  - Only happens every 100 iterations

```
if constexpr (with_residual) {
  residual = mpi::all_reduce(cart, residual, std::plus<>{});
  return residual;
}
```

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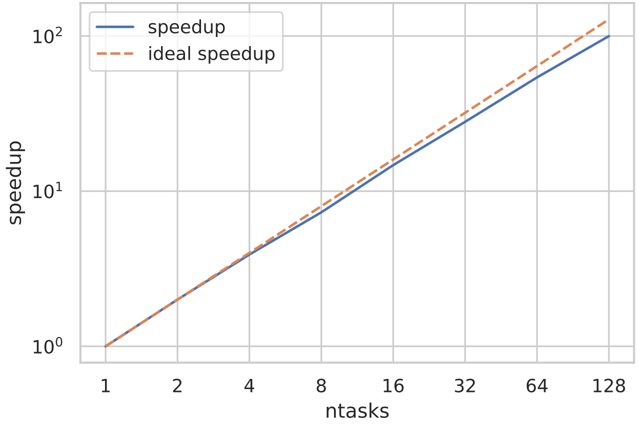
- Strong Scaling
- Weak Scaling
- Vampir

Strong scaling

- Strong scaling tests made with 2500x2500 grid
- 1, 2, 4, 8, 16, 32, 64 and 128 threads
- 128 threads on more than one node

Strong scaling graph

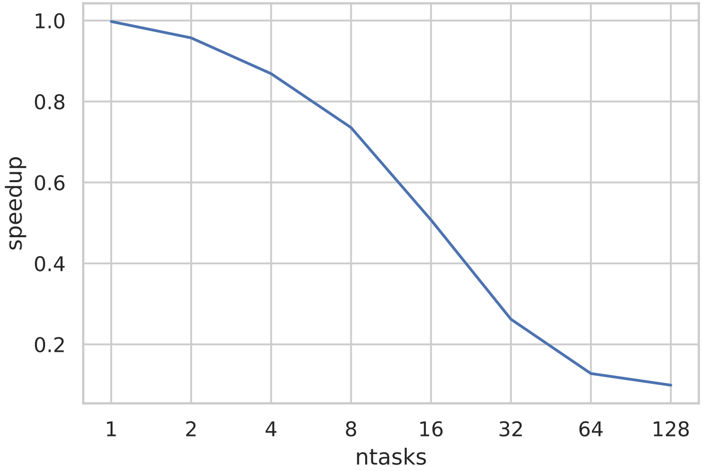
- 128 Tasks: $99/128 = 0.778$



Weak scaling

- Also 1, 2, 4, 8, 16, 32, 64 and 128 tasks
- Iterations are fixed at 20000
- $n^2 = 1000^2 \cdot \text{tasks}$
- $n = 1000 \cdot \sqrt{\text{tasks}}$

Weak scaling graph



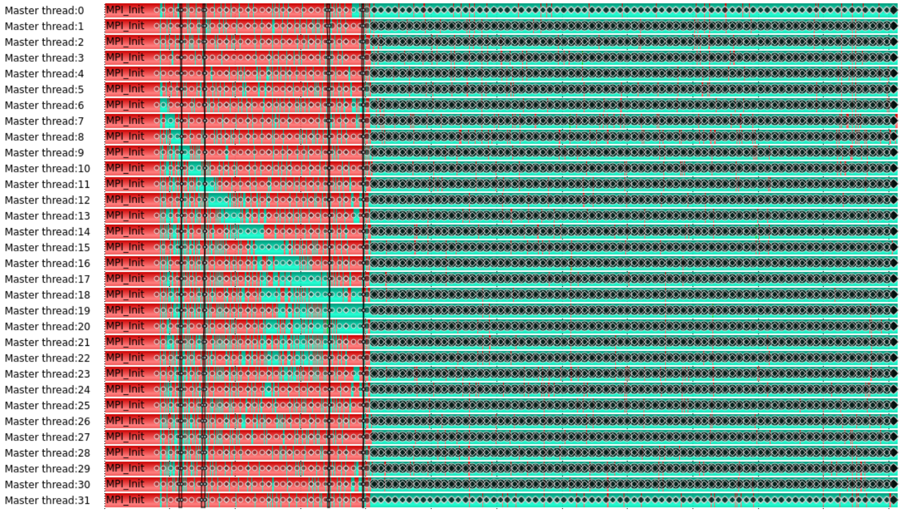
Interpretation

- $2 \cdot \text{test}_{16} \approx \text{test}_{32}$
- Suboptimal grid division
  - per task communication $\propto n$

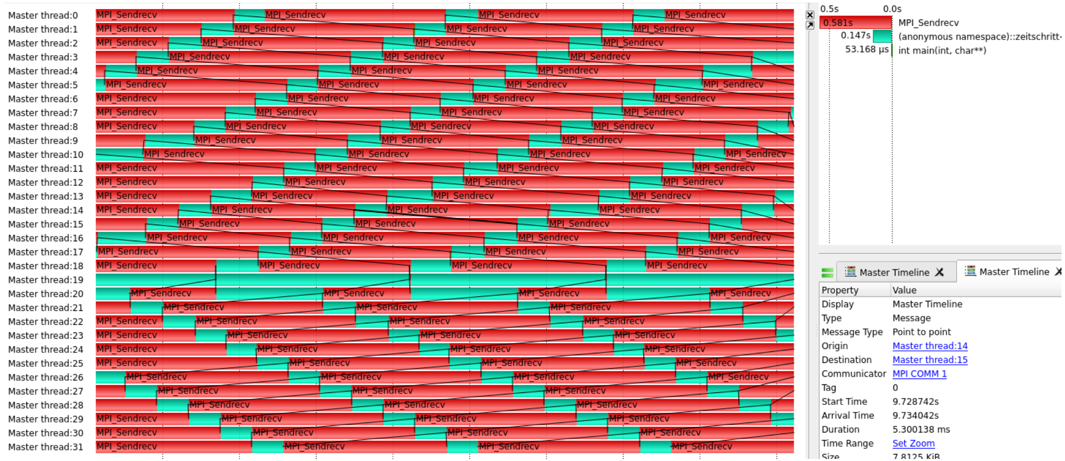
Scorep

- 32 task experiment
- Scorep instrumentation
- Profile
  - 70.2% in zeitschritt without residual
  - 20.5% in MPI_Sendrecv
  - 0.7% in zeitschritt with residual
- Run with tracing

Vampir


Master thread:0
Master thread:1
Master thread:2
Master thread:3
Master thread:4
Master thread:5
Master thread:6
Master thread:7
Master thread:8
Master thread:9
Master thread:10
Master thread:11
Master thread:12
Master thread:13
Master thread:14
Master thread:15
Master thread:16
Master thread:17
Master thread:18
Master thread:19
Master thread:20
Master thread:21
Master thread:22
Master thread:23
Master thread:24
Master thread:25
Master thread:26
Master thread:27
Master thread:28
Master thread:29
Master thread:30
Master thread:31
MPI_Init

Vampir



🟥 0.581s	MPI_Sendrecv
🟩 0.147s	(anonymous namespace)::zeitschritt·
53.168 μs	int main(int, char**)

Property	Value
Display	Master Timeline
Type	Message
Message Type	Point to point
Origin	Master thread:14
Destination	Master thread:15
Communicator	MPI COMM 1
Tag	0
Start Time	9.728742s
Arrival Time	9.734042s
Duration	5.300138 ms
Time Range	Set Zoom
Size	7.8125 KiB

Denormalized Floating Point

```cpp
auto grid_point_step(float a, float b, float c, float d, float prev_result) {
  const auto average = (a + b + c + d) / 4;
  const auto result = prev_result + 1.7 * (average - prev_result);
  return result;
}
static void normal(benchmark::State& state) {
  volatile float a = 1;
  volatile float b = 1;
  volatile float c = 1;
  volatile float d = 1;
  volatile float prev_result = 1;
  for (auto _ : state) {
    const auto result = grid_point_step(a, b, c, d, prev_result);
    benchmark::DoNotOptimize(result);
  }
}
```

Denormalized Floating Point

```
static void neighbors_denormal(benchmark::State& state) {
  volatile float a = std::numeric_limits<float>::denorm_min();
  volatile float b = std::numeric_limits<float>::denorm_min();
  volatile float c = std::numeric_limits<float>::denorm_min();
  volatile float d = std::numeric_limits<float>::denorm_min();
  volatile float prev_result = 1;
  for (auto _ : state) {
    const auto result = grid_point_step(a, b, c, d, prev_result);
    benchmark::DoNotOptimize(result);
  }
}
```

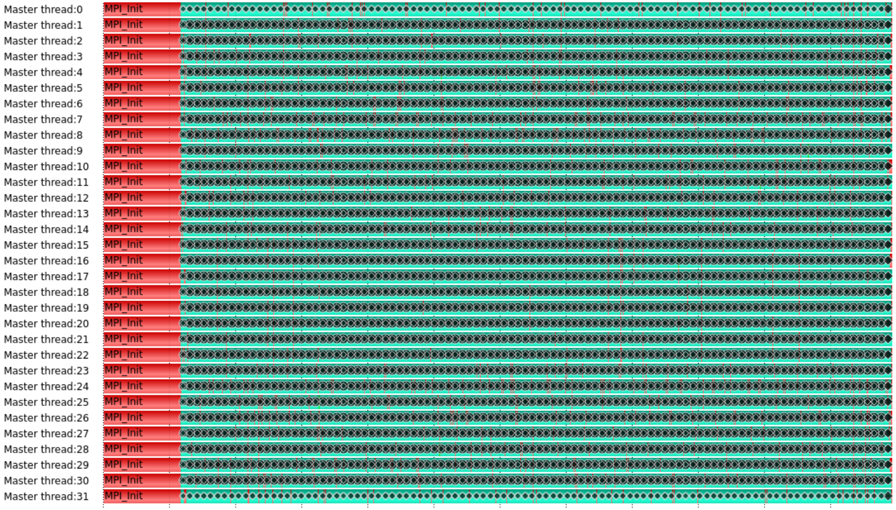
Denormalized Floating Point

- normal: 1.95 ns
- neighbors_denormal: 50.9 ns
- simple fix: $\text{initial guess} = 1$
- 28s$\rightarrow$21s

Improved Vampir profile

- 85.7% in zeitschritt without residual
- 9.8% in MPI_Init
- 3.0% in MPI_Sendrecv
- 0.9% in zeitschritt with residual

Improved Vampir profile



Conclusion

- Goals achived?

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  - Yes!

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- Lots of Performance improvements

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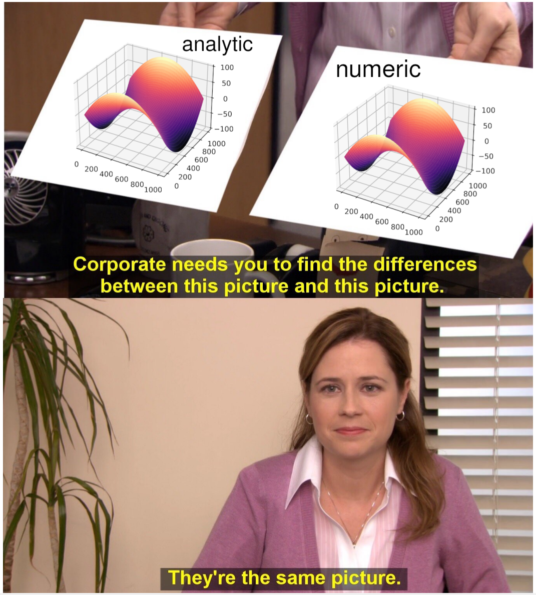
- n-Dimensional

Conclusion

- Goals achived?
  - Yes!
- Lots of Performance improvements
- n-Dimensional
- Input-file


analytic
numeric
100
50
0
−50
−100
0
200
400
600
800
1000
Corporate needs you to find the differences between this picture and this picture.
They're the same picture.