CS 294-73
Software Engineering for Scientific Computing

Homework Assignment 5 (and a little more)

Multigrid

$$
\begin{aligned}
&vcycle(\phi, \rho)\\
&\{\\
&\quad \phi := \phi + \lambda(L(\phi) - \rho)\ p \text{ times}\\
&\quad \text{if } (level > 0)\\
&\quad \{\\
&\qquad \mathcal{R} = \rho - L(\phi)\\
&\qquad \mathcal{R}_c = \mathcal{A}(\mathcal{R})\\
&\qquad \delta : B_c \rightarrow \mathbb{R}\ ,\ \delta = 0\\
&\qquad vcycle(\delta, \mathcal{R}_c)\\
&\qquad \phi := \phi + \mathcal{I}(\delta)\\
&\qquad \phi := \phi + \lambda * (L(\phi) - \rho)\ p \text{ times}\\
&\quad \}\\
&\quad \text{else}\\
&\quad \{\\
&\qquad \phi := \phi + \lambda * (L(\phi) - \rho)\ p_B \text{ times}\\
&\quad \{\\
&\}
\end{aligned}
$$

At the top level, iterate until residual is reduced by some large factor.

Baseline implementation of Residual

```
Multigrid::residual(...)
{
...
res.setVal(0.);
for (Point pt=bx.getLowCorner();bx.notDone(pt);bx.increment(pt))
  {
    for (int dir = 0; dir < DIM ; dir++)
      {
          Point edir = getUnitv(dir);
          res[pt] += (a_phi[pt + edir] + a_phi[pt-edir]);
       }
    res[pt] = res[pt]*dimqtr + .5*a_phi[pt];
}
for (Point pt=bx.getLowCorner();bx.notDone(pt);bx.increment(pt))
{
    a_phi[pt] = res[pt] - m_lambda*a_rhs[pt];
}
```

Getting timer output

```
> setenv CH_TIMER
> printenv
...
CH_TIMER =
> ./mg2D.exe < infile
...
total flops = 93148718
```

And we look at `time.table`

```
-----------------------------------------------------
[2]mg 0.36704 13
    100.0%  0.3670       13 vcycle [3]
    100.0%                  Total
-----------------------------------------------------
[3]vcycle 0.36703 13
    64.1%  0.2354       26 relax [4]
    24.8%  0.0910       13 vcycle [5]
     5.5%  0.0203       13 residual [10]
     2.7%  0.0101       13 avgdown [12]
     2.7%  0.0099       13 fineInterp [13]
    99.9%                  Total
-----------------------------------------------------
```

Is this good or bad ? 93148718 / .367 = 254 Mflops (not good).

Replace Baseline Implementation with Pencils

```
-----------------------------------------------------
[2]mg 0.34756 13
    100.0%  0.3475       13 vcycle [3]
    100.0%                  Total
-----------------------------------------------------
[3]vcycle 0.34753 13
    69.2%  0.2405       26 relax [4]
    24.2%  0.0839       13 vcycle [5]
     3.0%  0.0106       13 avgdown [9]
     2.6%  0.0090       13 fineInterp [11]
     0.9%  0.0033       13 residual [14] (vs. 0.0203)
    99.9%                  Total
-----------------------------------------------------
```

(1) Good news: looks like we reduce the run time by 6X.

(2) We haven't gotten the big pieces; Furthermore, even after we get `relax`, `avgdown` and `fineInterp` start to look relatively large.

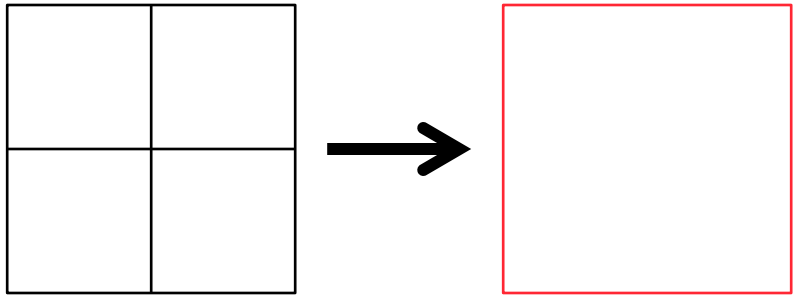
Replace Baseline Implementation with Pencils

```
-----------------------------------------------------
[2]mg 0.06940 13
    100.0%  0.0694       13 vcycle [3]
    100.0%                  Total
-----------------------------------------------------
[3]vcycle 0.06940 13
    39.4%  0.0274       26 relax [4] (vs. 0.2405)
    26.1%  0.0181       13 vcycle [6]
    15.6%  0.0108       13 fineInterp [7]
    14.5%  0.0101       13 avgdown [9]
     4.0%  0.0028       13 residual [14] (vs. 0.0203)
    99.6%                  Total
-----------------------------------------------------
```

(1) `avgdown` and `fineInterp` are now 20% of the time, so we probably want to get them, if it is not too painful.

Baseline implementation of avgdown

```
Multigrid::residual(...)
{
...
DBox bxKernel(getZeros(),getOnes());
double normalize = 1.0/bxKernel.sizeOf();
for (Point ptc = bxc.getLowCorner();bxc.notDone(ptc);
     bxc.increment(ptc))
    {
      for (Point ptsten = getZeros();bxKernel.notDone(ptsten);
           bxKernel.increment(ptsten))
        {
          a_resc[ptc] += a_res[ptc*2 + ptsten];
        }
      a_resc[ptc]*=normalize;
    }
}
```



Timing subsections

You need to know how you are doing at the small scale. You can time subsections, but you need to count the flops as well. Modify the flop counters, and add member data

```
Multigrid::vCycle(...)
{...
  pointRelax(a_phi,a_rhs,m_preRelax);
  m_flops += m_preRelax*m_box.sizeOf()*(2*DIM + 5);
  if (m_level > 0)
    {
      residual(m_res,a_phi,a_rhs);
      m_flops += m_box.sizeOf()*(2*DIM + 4);
      avgDown(m_resc,m_res);
      m_flops += m_box.sizeOf();
      m_delta.setVal(0.);
      m_coarsePtr->vCycle(m_delta,m_resc);
      fineInterp(a_phi,m_delta);
      m_flops += m_box.sizeOf();
      pointRelax(a_phi,a_rhs,m_postRelax);
      m_flops += m_postRelax*m_box.sizeOf()*(3*DIM + 3); ...
```

Timing subsections

You need to know how you are doing at the small scale. You can time subsections, but you need to count the flops as well. Modify the flop counters, and add member data

```
Multigrid::vCycle(...)
{...
  pointRelax(a_phi,a_rhs,m_preRelax);
  m_flops += m_preRelax*m_box.sizeOf()*(2*DIM + 5);
  if (m_level > 0)
    {
      residual(m_res,a_phi,a_rhs);
      m_flops += m_box.sizeOf()*(2*DIM + 4);
      avgDown(m_resc,m_res);
      m_flops += m_box.sizeOf();
      m_delta.setVal(0.);
      m_coarsePtr->vCycle(m_delta,m_resc);
      fineInterp(a_phi,m_delta);
      m_flops += m_box.sizeOf();
      pointRelax(a_phi,a_rhs,m_postRelax);
      m_flops += m_postRelax*m_box.sizeOf()*(3*DIM + 3); ...
```

Squeezing performance out

Vectorization

Using `clang`:

```
CFLAGS += -Rpass=loop-vectorize
```

If you want to know what loops are failing to vectorize, and why,

```
CFLAGS += -Rpass-analysis=loop-vectorize
```

Using `g++`:

```
CFLAGS+=-ftree-vectorizer-verbose=2
```

To turn off vectorization:

```
CFLAGS += -fno-vectorize
```

(However, g++ is more pessimistic about the value of vectorization).

Vectorization

Using `clang:`

`CFLAGS += -Rpass=loop-vectorize` - tells you what loops vectorize

If you want to know what loops are failing to vectorize, and why,

`CFLAGS += -Rpass-analysis=loop-vectorize`

Using `g++:`

`CFLAGS+=-ftree-vectorizer-verbose=2`

To turn off vectorization:

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(However, g++ is more pessimistic about the value of vectorization).

Pencils only work if unambiguous

```
double* a,b,c,d;
...
for (int k = 0; k < bar.size(); k++)
 {
   a[k] = b[k] * c[k] + d[2*k];
 }
```

Fails. Instead, use

```
double* a,b,c;
...
int high = bar.size();
for (int k = 0; k < high; k++)
 {
   a[k] = b[k] * c[k] + d[2*k];
 }
```

Loop bodies have to have obvious constant-stride access, fixed loop limits.
If we replace `double* a,b,c,d;` with `vector a,b,c,d;`
will the compiler recognize the unit stride access ?

An Embedded Domain-Specific Language

$$
\begin{array}{l}
vcycle(\phi, \rho) \\
\{ \\
\quad \phi := \phi + \lambda(L(\phi) - \rho) \ p \text{ times} \\
\quad \text{if } (level > 0) \\
\quad \{ \\
\qquad \mathcal{R} = \rho - L(\phi) \\
\qquad \mathcal{R}_c = \mathcal{A}(\mathcal{R}) \\
\qquad \delta : B_c \rightarrow \mathbb{R} \ , \ \delta = 0 \\
\qquad vcycle(\delta, \mathcal{R}_c) \\
\qquad \phi := \phi + \mathcal{I}(\delta) \\
\qquad \phi := \phi + \lambda * (L(\phi) - \rho) \ p \text{ times} \\
\quad \} \\
\quad \text{else} \\
\quad \{ \\
\qquad \phi := \phi + \lambda * (L(\phi) - \rho) \ p_B \text{ times} \\
\quad \{ \\
\}
\end{array}
$$

At the level of vcycle our code looks like this, but inside it is messy, particularly when you start optimizing for performance.

Can we do better ?

- Identify programming abstractions corresponding to the high-level mathematical abstractions.
- Implement as a library that curates the optimizations you do by hand.
- (apply compiler technologies to make it even better).

An Embedded Domain-Specific Language

At the level of vcycle our code looks like our pseudocode, but inside it is messy, particularly when you start optimizing for performance.

Can we do better ?

- Identify programming abstractions as aggregate operations corresponding to the high-level mathematical abstractions.
- Implement as C++ classes that contain the optimizations you would otherwise do by hand. The idea is that the opportunities for obtaining high performance come from the mathematical structure of the algorithms.
- (apply compiler technologies to make it even better).

`RectMDArray` does half of this, i.e. defines high-level data structures. We'll now take a look at the other half of the `RectMDArray` infrastructure, which is a stencil language.

(Joint work with Brian Van Straalen, Chris Gebhart).

Stencil Operators

$$\phi : B \rightarrow \mathbb{R}^N \ , \ B \text{ a } \texttt{Box}$$

$$L(\phi)_{\boldsymbol{i}} = \sum_{\boldsymbol{s} \in \mathcal{S}} a_{\boldsymbol{s}} \phi_{\boldsymbol{i}+\boldsymbol{s}} \ , \ \boldsymbol{i} \in B'$$

Can think of the operator L as an object that acts any `RectMDArray`.

$$L = \sum_{\boldsymbol{s} \in \mathcal{S}} a_{\boldsymbol{s}} S^{\boldsymbol{s}} \ , \ S^{\boldsymbol{s}}(\phi)_{\boldsymbol{i}} = \phi_{\boldsymbol{i}+\boldsymbol{s}}$$

Stencil operators have their own algebra: you can add them, compose them, multiply them by scalars, without knowing the details of what they will be applied to.

$$L_{1,2} = \sum_{\boldsymbol{s} \in \mathcal{S}} a^{1,2}_{\boldsymbol{s}} S^{\boldsymbol{s}}$$

$$L_1 \circ L_2 = \sum_{\boldsymbol{t}} (\sum_{\boldsymbol{s}+\boldsymbol{s}'=\boldsymbol{t}} a^1_{\boldsymbol{s}} a^2_{\boldsymbol{s}'}) S^{\boldsymbol{t}}$$

Stencil Operators

```
Stencil<double > m_Lap2nd;

m_Lap2nd =
       Stencil<double>(2.0*DIM)*Shift(getZeros());

    for (int dir = 0; dir < DIM ; dir++)
    {
        Point edir = getUnitv(dir);
        Stencil<double> plus = 1.0*Shift(edir);
        Stencil<double> minus = 1.0*Shift(edir*(-1));

        m_Lap2nd = m_Lap2nd + minus + plus;
    }
```

Stencil Operators

```
Multigrid::residual(
                    RectMDArray<double >& a_res,
                    RectMDArray<double >& a_phi,
                    RectMDArray<double >& a_rhs
                    )
{
  CH_TIMERS("residual");
  DBox bx = m_box;
  getGhost(a_phi);
  double hsqi = 1.0/(m_dx*m_dx);
  a_res|=m_Lap2nd(a_phi,bx,-hsqi);
  a_res += a_rhs;
};
```

DBox over which operator is applied.

Apply the operator and store in the lhs.

Stencil Operators

Stencils can be strided, both on input and on output. Useful for coarsening / refinement.

$$\mathcal{L}(\phi)_{ir^{dest}+q^{dest}} = \sum_{s} a_s \phi_{ir^{src}+s}, i \in \Gamma$$

Arithmetic on `RectMDArrays`

```
...
  a_res += a_rhs;
...
```

Defined on intersection of the two `DBoxes`.

Pointwise operators.

$$(f@(U))_{\boldsymbol{i}} \equiv f(U)_{\boldsymbol{i}} \ , \boldsymbol{i} \in B$$

```
forall(fOfU,U,f,bx); // f = f(U_in,U_out).
```

we can also use use lambda calculus in C++11 to apply partially evaluated functions.

```
forall(fOfU,U,[dt](State& a,const State& b){return f(a,b,dt);), bx);
```

Use lambdas to apply member functions of a class.

```
forall(W, U,
[this](State& a, const State& b){return consToPrim(a,b);}, B_3);
```

How do we get performance ?

In the apply function, we implement the pencil construction once.

```
...
for (int isten =0;isten < srcOffset.size(); isten++)
{
   int kpoffset = kbasep+srcOffset[isten];
   double coefpt = coef[isten];
   for (int k0 = 0;k0 < nptsDst;k0++)
    {
     const T& phival = (phi_ptr_i)[kpoffset+k0];
     T& lofphi = (lofphi_ptr_i)[kbasel+k0];
     lofphi+=coefpt*phival;
     }
}
...
```

How is the performance ?

```
-----------------------------------------------------
[2]mg 0.07775 13
    100.0%  0.0777       13 vcycle [3]
    100.0%                  Total
-----------------------------------------------------
[3]vcycle 0.07774 13 (compare to .347 baseline, .056 by hand).
    58.5%  0.0455       26 relax [4]
    28.5%  0.0222       13 vcycle [8]
     6.4%  0.0050       13 residual [16]
     3.4%  0.0027       13 fineInterp [24]
     2.7%  0.0021       13 avgdown [30]
    99.6%                  Total
-----------------------------------------------------
```

i.e. we get about 1.2 Gflops from stencil, vs. 1.7 Gflops by hand, and 268 Mflops baseline.

- This is respectable. If we want to get the last 40% on a few performance-critical sections, we can tune those by hand.
- There is another advantage to stencils, which is productivity. It is actually better than the baseline (and of the hand-tuned), from that standpoint.

Multigrid in a slide

```
// residual.
a_res|=m_Lap2nd(a_phi,bx,-hsqi);
a_res += a_rhs;

// pointRelax:
for (int iter = 0; iter < a_numIter; iter++)
    {
      getGhost(a_phi);
      {lofphi |= Identity(a_rhs,m_box,-m_lambda);
       lofphi += m_Jacobi(a_phi,m_box);
       lofphi.copyTo(a_phi);}
    }

// fineInterp:
for (Point ptsten = Point::getZeros();
       m_boxSten.notDone(ptsten);m_boxSten.increment(ptsten))
    {a_phi += m_Interp(ptsten,0)(a_delta,bxc);}

//avgdown:
  DBox bxc = a_resc.getDBox();
  a_resc|=m_avgDown(a_res,bxc);
```

Stencils can be curated in a library.

```
//List of Implemented Stencils

        STRING:                 DESCRIPTION
        ------------------------------------------------
        Identity:               Trivial identity calculation
        FirstDeriv_2C[DIM]:     First Derivative,   2nd Order,  Centered
        FirstDeriv_2L[DIM]:     First Derivative,   2nd Order,  Low Edge
        FirstDeriv_2H[DIM]:     First Derivative,   2nd Order,  High Edge
        FirstDeriv_4C[DIM]:     First Derivative,   4th Order,  Centered
        FirstDeriv_4L[DIM]:     First Derivative,   4th Order,  Low Edge
        FirstDeriv_4H[DIM]:     First Derivative,   4th Order,  High Edge
        SecondDeriv_4C[DIM]:    Second Derivative,  4th Order,  Centered
        Laplacian_2:            Laplacian,          2nd Order
        Laplacian_19:           Laplacian,                      19 Point (3D)
        Laplacian_27:           Laplacian,                      27 Point (3D)
        Laplacian_117:          Laplacian,                      117 Point (3D)
        EdgeToCell_4[DIM]:      Edge->Cell Interp,  4th Order
        EdgeToCell_6[DIM]:      Edge->Cell Interp,  6th Order
        CellToEdge_5L[DIM]:     Cell->Edge Interp,  5th Order, Low Edge
        CellToEdge_5H[DIM]:     Cell->Edge Interp,  5th Order, High Edge
        CellToEdge_7L[DIM]:     Cell->Edge Interp,  7th Order, Low Edge
        CellToEdge_7H[DIM]:     Cell->Edge Interp,  7th Order, High Edge
        CellToEdge_9L[DIM]:     Cell->Edge Interp,  9th Order, Low Edge
        CellToEdge_9H[DIM]:     Cell->Edge Interp,  9th Order, High Edge
        FluxDivergence[DIM]:    Flux Differencing
```

Stencils can be curated in a library.

```
Multigrid::define(...)
{
...
  m_Lap2nd = SLib::get("Laplacian_2");
  m_Jacobi = m_Lap2nd;
  m_Jacobi = (4.0*DIM)*Shift(Point::getZeros()) + m_Jacobi;
  m_Jacobi*=1.0/(4.0*DIM);
  m_avgDown = SLib::get("AvgDown2");
  m_boxSten=DBox(Point::getZeros(),Point::getOnes());
  m_Interp.define(m_boxSten);
  for (Point pt =
Point::getZeros();m_boxSten.notDone(pt);m_boxSten.increment(pt))
    {
      m_Interp(pt,0) = (1.0)*Shift(Point::getZeros());
      m_Interp(pt,0).setDestRefratio(Point::getOnes()*2);
      m_Interp(pt,0).setDestShift(pt);
    }
...
```

Summary

- Small constant stride 1 access (e.g. stride 1), vectorization, make a big performance difference.
- You will find that doing by hand is drudgery.
- Higher-level abstractions can enable performance engineering by making them reuseable. Also allows you to improve performance without rewriting large amounts of application code.
- (Stencil library is available for use in structured grid projects, if anyone is feeling adventurous).