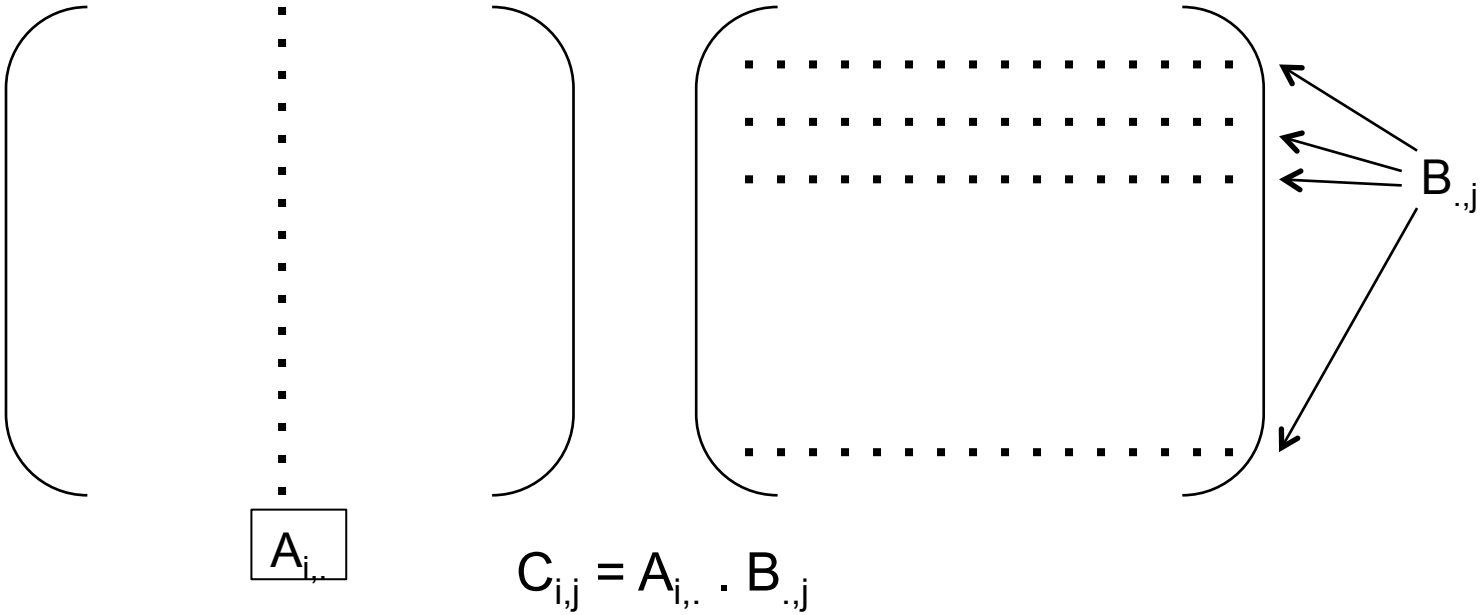
CS 294-73
Software Engineering for Scientific Computing

Lecture 17: Homework #4

Matrix multiplication and L3 cache

From last week



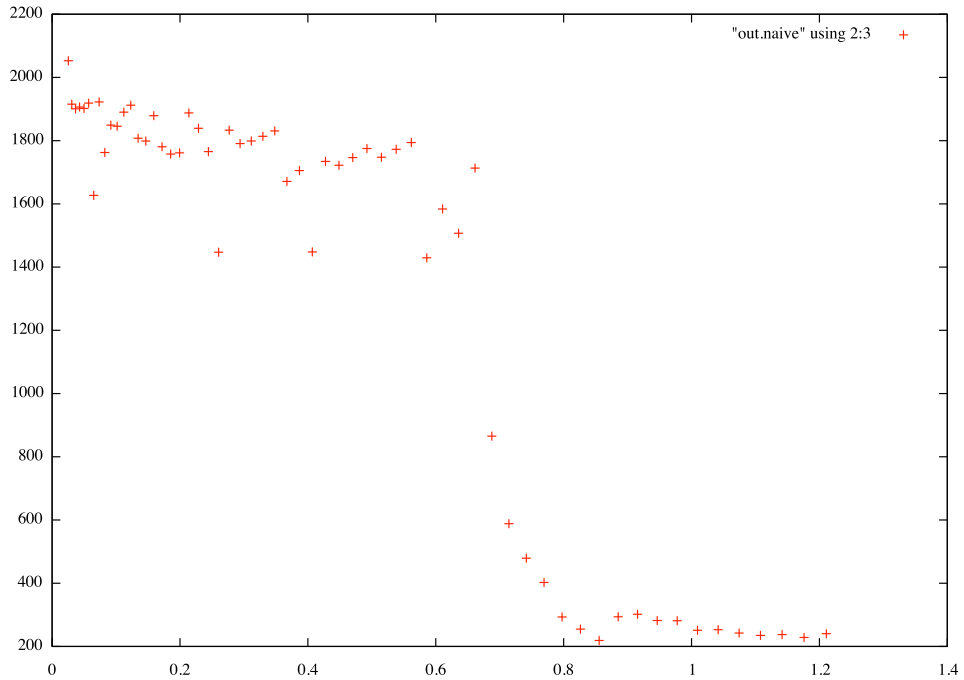
Triply-nested loop: for each column of A, cycle through all the rows of B to compute a column of C.

A simple cache-eviction policy: oldest (i.e. least-recently used) data gets overwritten when you run out of space.

Two possibilities: if B fits in cache, read it from main memory once. If not, you are always reading it from main memory.

Matrix multiplication and cache

Plot of performance as a function of (size of one matrix)/(size of L3). Here, the size of L3 is 3 MB.



This is actually pretty good for a simple cartoon of cache behavior.

Theorem says that you will always have this behavior for triply-nested loops.

Homework 4

PIC methods for vorticity.

- Algorithmic issues
- Software / implementation.

Regularized particle methods

Particle method for vorticity transport in 2D.

$$\frac{d\boldsymbol{x}^k}{dt} = \vec{U}(\boldsymbol{x}^k(t)) \qquad \omega^k = \omega(\boldsymbol{x}^k(0), 0)h^D$$

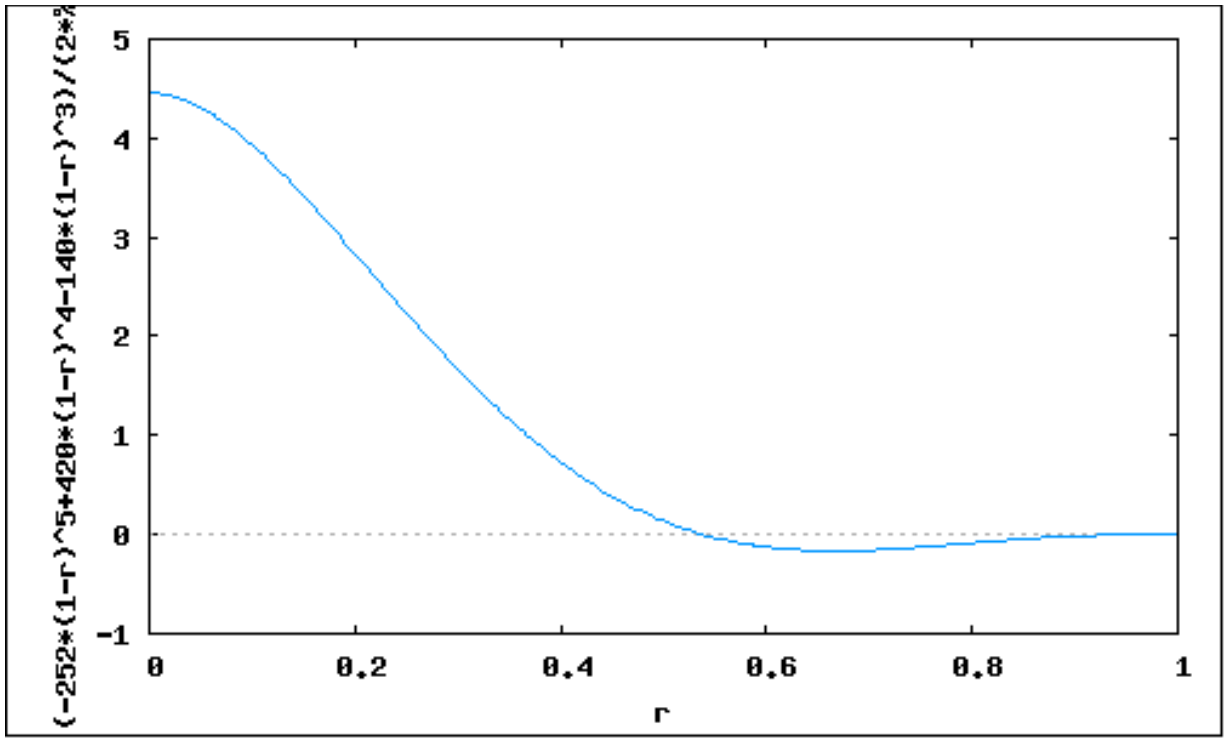
$$\vec{U}(\boldsymbol{x}) = \sum_k \omega^k \nabla_{\boldsymbol{x}}^{\perp} \int G(\boldsymbol{x}-\boldsymbol{y})\zeta_\epsilon(\boldsymbol{y})d\boldsymbol{y} \qquad G(\boldsymbol{z}) = \frac{1}{2\pi} log(|\boldsymbol{z}|)$$

$$= \sum_k \omega^k \vec{U}_\epsilon(\boldsymbol{x}-\boldsymbol{x}_k) \qquad \nabla_{\boldsymbol{x}}^{\perp} = (\frac{\partial}{\partial x_2}, -\frac{\partial}{\partial x_1})$$

$$U_\epsilon(\boldsymbol{z}) = \nabla_{\boldsymbol{z}}^{\perp}\Big(\int G(\boldsymbol{z}-\boldsymbol{y})\zeta_\epsilon(\boldsymbol{y})d\boldsymbol{y}\Big) \qquad \zeta_\epsilon(\boldsymbol{z}) = \frac{1}{\epsilon^D}\zeta(\frac{\boldsymbol{z}}{\epsilon})$$

For epsilon = 0, we get a point vortex method, with a singular velocity field, so some sort of regularization (epsilon > 0) is required.

Regularized particle methods



$$\zeta(z) = \frac{(-140(1-|z|)^3 + 420(1-|z|)^4 - 252(1-|z|)^5)}{2\pi}$$

Regularized particle methods

Can think of this as regularizing the potential induced by a collection of delta functions.

$$\omega(\boldsymbol{x}) = \sum_k \omega_k \delta(\boldsymbol{x} - \boldsymbol{x}_k)$$

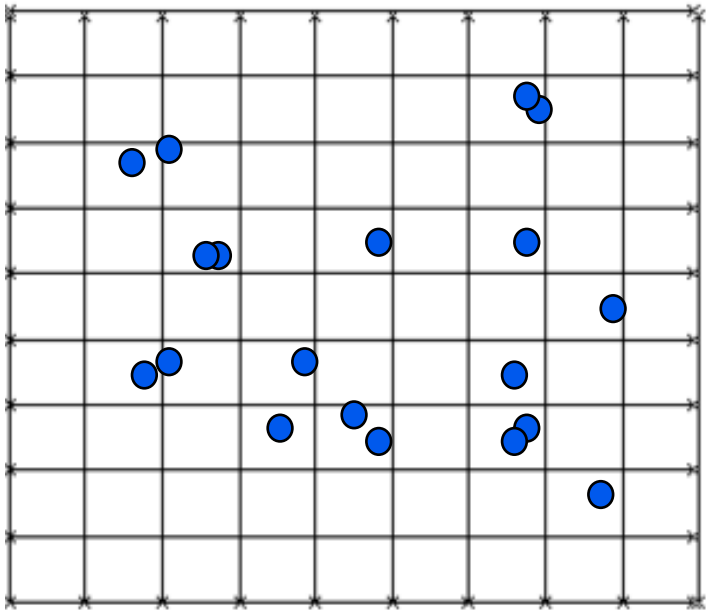
$$\Psi(\boldsymbol{x}) = (G * \omega)(\boldsymbol{x}) = \sum_k \omega_k G(\boldsymbol{x} - \boldsymbol{x}_k) \ ,$$

$$\Downarrow$$

$$\Psi(\boldsymbol{x}) = (G_\epsilon * \omega)(\boldsymbol{x}) = \sum_k \omega_k G_\epsilon(\boldsymbol{x} - \boldsymbol{x}_k)$$

$$U = \nabla^\perp \Psi$$

Particle-in-Cell (PIC)



Start with a collection of particles, each of which induces a contribution to the stream function in any point in space via convolution.

PIC: Replace continuous convolution with discrete convolution on a rectangular grid:

- Replace $\omega_k \delta(\boldsymbol{x} - \boldsymbol{x}_k) \rightarrow \omega_{\boldsymbol{i}} += \omega_k \delta^h(\boldsymbol{i}h - \boldsymbol{x}_k)$
- Compute stream function on the grid as discrete convolution.
- Interpolate finite-difference approximation to velocity on the grid to particles.

Particle-in-Cell (PIC)

Given the particle locations, can compute a velocity field at those locations.

$$\omega_i = \sum_k \omega^k \delta_h(ih - x^k) \ , \ \omega^k = \omega^k(x^k(0), 0)$$ Deposition

$$\psi_i = \sum_j G(ih - jh)\omega_j \qquad G(z) = \frac{1}{2\pi} log(|z|)$$ Discrete convolution

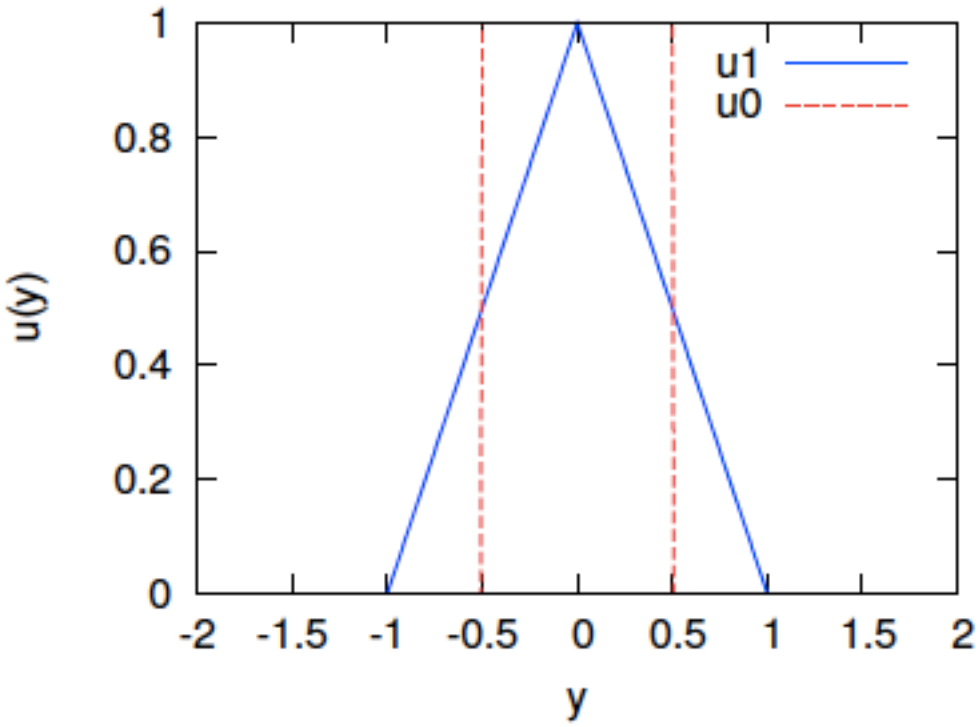
$$\vec{U}_i = D^{\perp}(\psi)_i$$

$$(D_1\psi) = \frac{\psi_{i+(1,0)} - \psi_{i-(1,0)}}{2h} \ , \ (D_2\psi) = \frac{\psi_{i+(0,1)} - \psi_{i-(0,1)}}{2h}$$ Grid velocity

$$U(x^k) = \sum_i U_i \delta_h(x^k - ih) \qquad \delta_h(z) = \delta(\frac{z_1}{h})\delta(\frac{z_2}{h})$$ Particle velocity

Particle-in-Cell (PIC)

$$U(x^k) = \sum_i U_i \delta_h(x^k - ih) \qquad \delta_h(z) = \delta(\frac{z_1}{h})\delta(\frac{z_2}{h})$$



Algorithmic design considerations

- Initialization: particles deposited on a grid with spacing h_p.
- What is the relationship between epsilon, h, h_p ? Our choices: $h_p = h/n_p$, n_p a positive integer, epsilon = h.
- There is a good convergence theory for vortex methods (i.e. no grid). The grid introduces its own short-range regularization. Can we eliminate that, while still retaining the (fast) grid representation of the long-range effects ? (Answer: yes - PPPM).

Division of Labor

We will provide an implementation of Hockney's algorithm for computing

$$\psi_i = \sum_j G_\epsilon(ih - jh)\omega_j$$

as well as the templated RK4 class.

You will implement the rest of the particle method:

- Deposition of charge and calculation of velocity field (template class `F`).
- The template classes `x, dx` appropriate to the PIC method.

RK4

```
template <class X, class F, class dX> class RK4
{
  public:  void advance(double a_time, double a_dt, X&
  a_state);
  protected:
  dX m_k;
  dX m_delta;
  F m_f;
};
```

Particle Classes

```
class DX // displacement.
{
public:
  DX()
  {...}
  array<Real, DIM> m_x;
  inline void increment(double a_scale, const DX& a_rhs)
  {...}
  inline void operator*=(double a_scale){...};
};
```

Particle Classes

```
class Particle
{
public:
  array<Real, DIM> m_x;
  Real strength;
  // (*this).m_x -> (*this).m_x + a_shift.m_x;
  inline void increment(const DX& a_shift)
  {...}
};
```

Particle Classes

```
class ParticleSet; // Forward declaration.
                   // Needed to avoid circular dependency.

class ParticleShift // Corresponds to dX in RK4.

{

public:

  vector<DX> m_particles;

  void init(const ParticleSet& a_particles);

  void increment(double a_scale, const ParticleShift& a_rhs);

  void operator*=(double a_scale);

  void setToZero();

};
```

All that the `ParticleShift` declaration is allowed to know about `ParticleSet` is that it is a class. Pointers, references, but *not* values (why?).

Particle Classes

```
class ParticleSet
// Corresponds to template class X in RK4.
{
Public:
  ParticleSet(shared_ptr<ConvKernel>& a_kerptr,
              Box& a_box,
              double& a_h,
               array<Real, DIM>& a_lowCorner,
              int a_M);
  ParticleSet(){};
  vector<Particle> m_particles;
  double m_h;
  Box m_box;
  array<Real, DIM> m_lowCorner;
  Hockney m_hockney;

  void increment(const ParticleShift& a_shift);
};
```

Particle Classes

```
class ParticleVelocities // Implements template class F
{
public:
  ParticleVelocities();
  void operator()(ParticleShift& a_k,
                  const Real& a_time, const Real& dt,
                  ParticleSet& a_state);
};
```

`ParticleVelocities` has no state, only a default constructor. All objects required to to evaluate the velocity must come in via `a_state`. This is one of the reasons why all of the member data of `ParticleSet` are public (alternative: friend classes).

Hockney Class

```
class Hockney
{public:
  Hockney();
  Hockney(shared_ptr<ConvKernel>& a_kerPtr,const double&
  a_h,int a_M);
  void define(shared_ptr<ConvKernel>& a_kerPtr,const
  double& a_h,int a_M);
  void convolve(RectMDArray<Real>& a_rhs);
  ~Hockney(){};
protected:
  ...
};
```

You will have to define your Hockney in the ParticleSet constructor. `a_kerptr`, `a_M`, and `a_h` are passed through to you via the arguments.

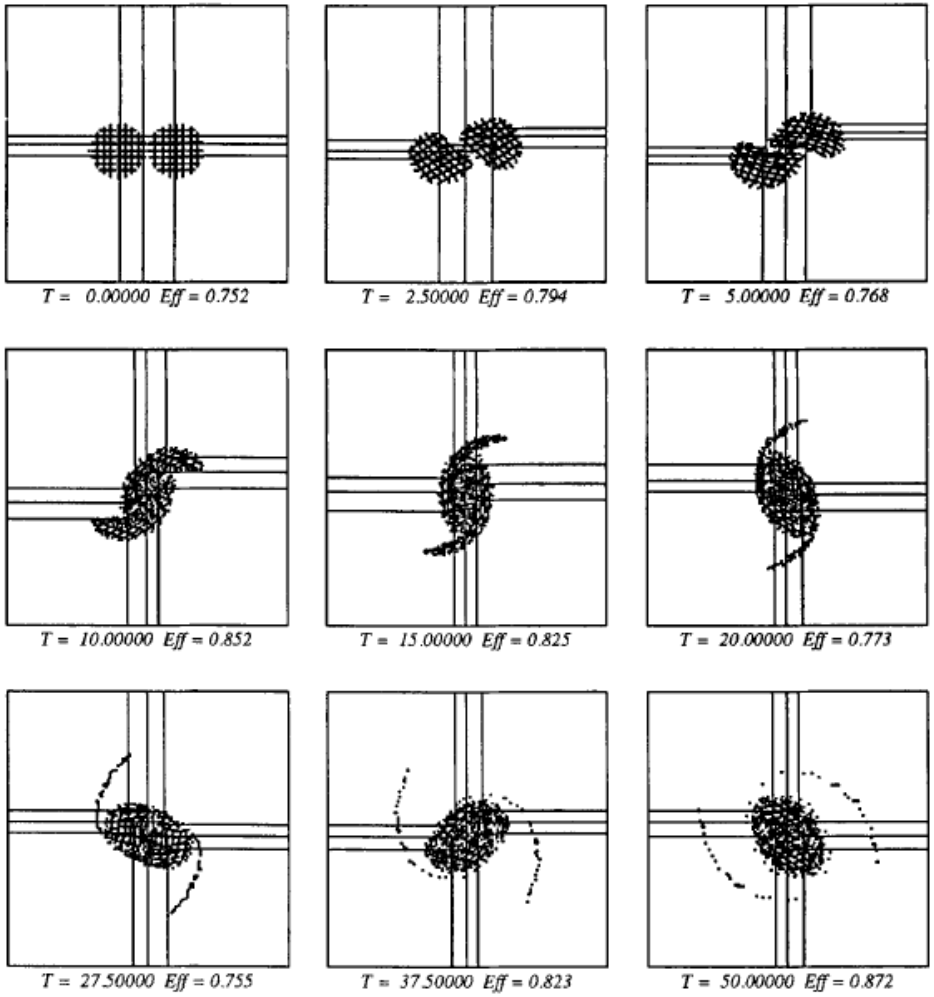
`m_hockney.convolve(...)` called in `ParticleVelocities`.

Programming ODE Methods

```
template <class X, class F, class dX>
void RK4<X,F,dX>::advance(double a_time, double a_dt, X& a_state)
{
  m_delta.init(a_state);
  m_k.init(a_state);
  m_f(m_k, a_time, a_dt, a_state, m_k);  // compute k1
  // F::operator()(dX&,double&,double&,X&,dX&);
  m_delta.increment(sixth, m_k);  m_k*=half;
  m_f(m_k, a_time+half*a_dt, a_dt, a_state, m_k); // compute k2
  m_delta.increment(third, m_k);  m_k*=half;
  m_f(m_k, a_time+half*a_dt, a_dt, a_state, m_k);  // conpute k3
  m_delta.increment(third, m_k);
  m_f(m_k, a_time+a_dt, a_dt, a_state, m_k); // compute k4
  m_delta.increment(sixth, m_k);
  a_state.increment(m_delta);
}
```

Initialize dX classes from a_state.

Test Problems



Visit for Particles

From the directory you ran vortex2d.exe:

- Visit
  - open -> PART*.vtk (database)
  - controls -> view -> 2D -> set viewport, window to 0 1 0 1, apply, dismiss
  - add -> mesh -> mesh
  - draw
  - For small number of particles: click on mesh, change point type to sphere, pixels to 10

Back to organization / make process

Top-level directory structure:

```
src/
    src/RectMDArray/
    src/fftTools/ - Contains only FFT1D, FFT1DW, FFTMD
    src/Particles/ – .H only – you will put your .cpp files here
    src/Hockney/
utils/
    utils/Writers/
    utils/timer/
exec/
```

exec/

```
exec/
    exec/GNUmakefile
    exec/vortexTest.cpp
    exec/o2d/
    exec/d2d/
```

Makefile will create `o2d/, d2d/` directories.

- `o2d/` will contain the `.o` files generated in the build process.
- `d2d/` will contain the `.d` files (dependencies) generated in the build process.

GNUmakefile

```
HOME = ./..
WRITERS = $(HOME)/utils/Writers
RMDA = $(HOME)/src/RectMDArray
FFT = $(HOME)/src/fftTools
CONV = $(HOME)/src/Hockney
PARTICLES = $(HOME)/src/Particles
TIMER = $(HOME)/utils/timer
VPATH= . $(HOME) $(PARTICLES) $(RMDA) $(FFT) $(CONV) $
(TIMER) $(WRITERS)
```

Tells Gmake where to search for file dependencies.

```
DIM=2
#CXX=g++
CXX=clang++
FFTWDIR = /usr/local
#CFLAGS = -g -Wall
CFLAGS = -O3
CFLAGS += -std=c++11 -I/. -I$(PARTICLES) -I$(RMDA) -I$
(FFT) -I$(CONV) -I$(TIMER) -I$(WRITERS) -I$(FFTWDIR)/
include
```

Tells the compiler where to look for `#include` files

```
CFLAGS += -D DIM=$(DIM)
```

GNUmakefile

```
odir = ./o.$(DIM)d
ddir = ./d.$(DIM)d

LIBS:=  -L$(FFTWDIR)/lib -lfftw3

SRCFILES:= $(notdir $(wildcard $(TIMER)/*.cpp $(RMDA)/
*.cpp $(WRITERS)/*.cpp $(FFT)/*.cpp ./*.cpp $(CONV)/*.cpp
$(PARTICLES)/*.cpp))
```

This defines our `.cpp` sources. `notdir` strips off the directory part of each element in the list.

```
OBJS:=$(patsubst %.cpp,$(odir)/%.o,$(SRCFILES))
```

This defines our object files. With this definition, make will look for them in `./$(odir)`

```
DEPS:=$(patsubst $(odir)/%.o,$(ddir)/%.d, $(OBJS))
```

This defines our dependency files to be stored in `$(ddir)`. More on them shortly.

GNUmakefile

```
odir = ./o.$(DIM)d
ddir = ./d.$(DIM)d

LIBS:=  -L$(FFTWDIR)/lib -lfftw3

SRCFILES:= $(notdir $(wildcard $(TIMER)/*.cpp $(RMDA)/
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```
DEPS:=$(patsubst $(odir)/%.o,$(ddir)/%.d, $(OBJS))
```

This defines our dependency files to be stored in `$(ddir)`. More on them shortly.

Rule for making .o files.

```
$(odir)/%.o:%.cpp GNUmakefile
<TAB>  mkdir -p $(odir); \
       $(CXX) -c $(CFLAGS) $< -o $@
<TAB>  mkdir -p $(ddir); \
      $(CXX) -MM $(CFLAGS) $< \
       | sed '1s/^/o.$(DIM)d\//' > $*.d ;\
       mv $*.d $(ddir)
```

For each file of the form `%.cpp` accessible in VPATH, it makes a target of the form `$(odir)/%.o . $(CXX) -c :` compile only, output object file to argument following –`o` . In this case, it is `$@.`

This rule also makes a file of the form `$*.d` and moves it to `$(ddir).` (`$*` is the *stem* of `%.cpp`).

`mkdir –p` creates a directory only if there isn't one.

Questions:

What do the `.d` files do for us?

What's that stuff in the middle ?

Rule for making .o files.

`-include $(DEPS)` — includes all of the files in `$(DEPS)`. In this case, that is all files of the form `d.2d/*.d` . Placed at the end of the makefile. Each file is a makefile, with one rule in it.

Let's look at `d.2d/Box.d`:

```
o.2d/DBox.o: ../src/RectMDArray/DBox.cpp ../src/RectMDArray/DBox.H \
  ../src/RectMDArray/Point.H ../src/RectMDArray/PointImplem.H
```

It is a rule for making `o.2d/DBox.o`. But it has no recipes. The effect of this is to add dependencies to already-existing ones (in this case, for `o.2d/DBox.o`).

Rule for making .o files.

```
<TAB> mkdir -p $(ddir);$(CXX) -MM $(CFLAGS) $< | sed '1s/^/o.
$(DIM)d\//' > $*.d;mv $*.d $(ddir)
```

- | : take output from stdout and stream it to stdin for the next program.
- sed : streaming editor for Unix systems. Uses similar commands to vi.
- > : take output from stdout and send it to file on rhs.
- mv : move the file.

Rule for building vortex2D.exe

```
vortex2D: GNUmakefile $(OBJS)
        $(CXX) $(CFLAGS) $(OBJS) $(LIBS) -o vortex$(DIM)D.exe
```

- It depends on the makefile and everything in the `$(OBJS)` list.
- The rule is to run the compiler with no `.cpp` files, so all it is doing is linking the object files (so `main` had better be there).

Housekeeping, utilities.

```
clean:
<TAB>  rm -r *.exe $(odir) $(ddir)
listsrc:
<TAB>  @echo $(SRCFILES)
listobj:
<TAB>  @echo $(OBJS)
listdep:
<TAB>  @echo $(DEPS)
```

Results Demo