

CLEF: A Framework for Solving Conservation-law Equations

Andrew McMurry

April 7, 2014

Finite volume method

$$U_t + \nabla \cdot F(U) = S(U) \quad (1)$$

Finite volume method

$$U_t + \nabla \cdot F(U) = S(U) \quad (1)$$

$$\bar{U}^i = \frac{1}{V^i} \int_{V^i} U dV \quad (2)$$

Finite volume method

$$U_t + \nabla \cdot F(U) = S(U) \quad (1)$$

$$\bar{U}^i = \frac{1}{V^i} \int_{V^i} U dV \quad (2)$$

$$\frac{1}{V^i} \int_{V^i} U_t dV + \frac{1}{V^i} \int_{V^i} \nabla \cdot F(U) dV = \frac{1}{V^i} \int_{V^i} S(U) dV \quad (3)$$

Finite volume method

$$U_t + \nabla \cdot F(U) = S(U) \quad (1)$$

$$\bar{U}^i = \frac{1}{V^i} \int_{V^i} U dV \quad (2)$$

$$\bar{U}_t^i + \frac{1}{V^i} \int_{V^i} \nabla \cdot F(U) dV = \frac{1}{V^i} \int_{V^i} S(U) dV \quad (3)$$

Finite volume method

$$U_t + \nabla \cdot F(U) = S(U) \quad (1)$$

$$\bar{U}^i = \frac{1}{V^i} \int_{V^i} U dV \quad (2)$$

$$\bar{U}_t^i + \frac{1}{V^i} \oint_{S^i} F(U) \cdot dS = \frac{1}{V^i} \int_{V^i} S(U) dV \quad (3)$$

Finite volume method

$$U_t + \nabla \cdot F(U) = S(U) \quad (1)$$

$$\bar{U}^i = \frac{1}{V^i} \int_{V^i} U dV \quad (2)$$

$$\bar{U}_t^i + \sum_j \left(\frac{A^j}{V^i} \right) \bar{F}^j(\bar{U}) = \frac{1}{V^i} \int_{V^i} S(U) dV \quad (3)$$

Finite volume method

$$U_t + \nabla \cdot F(U) = S(U) \quad (1)$$

$$\bar{U}^i = \frac{1}{V^i} \int_{V^i} U dV \quad (2)$$

$$\bar{U}_t^i + \sum_j \left(\frac{A^j}{V^i} \right) \bar{F}^j(\bar{U}) = \bar{S}^i(\bar{U}) \quad (3)$$

Goals of the Framework

- ▶ Promote code re-use

Goals of the Framework

- ▶ Promote code re-use
- ▶ Support a library of standard algorithms

Goals of the Framework

- ▶ Promote code re-use
- ▶ Support a library of standard algorithms
- ▶ Avoid implementation specific dependencies

Goals of the Framework

- ▶ Promote code re-use
- ▶ Support a library of standard algorithms
- ▶ Avoid implementation specific dependencies
- ▶ Standard interfaces for algorithm types

Goals of the Framework

- ▶ Promote code re-use
- ▶ Support a library of standard algorithms
- ▶ Avoid implementation specific dependencies
- ▶ Standard interfaces for algorithm types
- ▶ Efficient executable

Problem

- ▶ The System of Equations

Problem

- ▶ The System of Equations
 - ▶ The Conserved Variables

Problem

- ▶ The System of Equations
 - ▶ The Conserved Variables
 - ▶ The Flux Function

Problem

- ▶ The System of Equations
 - ▶ The Conserved Variables
 - ▶ The Flux Function
 - ▶ Extra Information for Riemann Solver

Problem

- ▶ The System of Equations
 - ▶ The Conserved Variables
 - ▶ The Flux Function
 - ▶ Extra Information for Riemann Solver
 - ▶ Source Terms

Problem

- ▶ The System of Equations
 - ▶ The Conserved Variables
 - ▶ The Flux Function
 - ▶ Extra Information for Riemann Solver
 - ▶ Source Terms
- ▶ The Initial Conditions

Problem

- ▶ The System of Equations
 - ▶ The Conserved Variables
 - ▶ The Flux Function
 - ▶ Extra Information for Riemann Solver
 - ▶ Source Terms
- ▶ The Initial Conditions
- ▶ Boundary Conditions

Method

- ▶ Domain Discretization

Method

- ▶ Domain Discretization
- ▶ Riemann Solver

Method

- ▶ Domain Discretization
- ▶ Riemann Solver
- ▶ Order of Accuracy

Method

- ▶ Domain Discretization
- ▶ Riemann Solver
- ▶ Order of Accuracy
- ▶ Methods for Source Terms

Sections

Problem

- ▶ The System of Equations
 - ▶ **The Conserved Variables**
 - ▶ The Flux Function
 - ▶ Extra Information for Riemann Solver
 - ▶ Source Terms
- ▶ The Initial Conditions
- ▶ Boundary Conditions

Method

- ▶ Domain Discretization
- ▶ Riemann Solver
- ▶ Order of Accuracy
- ▶ Methods for Source Terms

The Conserved Variables - Traditional Implementation

```
double r[NX][NY][NZ];
double rux[NX][NY][NZ];
double ruy[NX][NY][NZ];
double ruz[NX][NY][NZ];
double E[NX][NY][NZ];

void forward_euler(double drdt, double druxdt, double druydt, double druzdt,
                  double dEdt, int i, int j, int k, double dt)
{
    r[i][j][k] = r[i][j][k] + dt * drdt;
    rux[i][j][k] = rux[i][j][k] + dt * druxdt;
    ruy[i][j][k] = ruy[i][j][k] + dt * druydt;
    ruz[i][j][k] = ruz[i][j][k] + dt * druzdt;
    E[i][j][k] = E[i][j][k] + dt * dEdt;
}
```

The Conserved Variables - Structural Implementation

```
class Variable {
public:
    double r;
    vector3 ru;
    double E;
};

Variable U[NX][NY][NZ];

void forward_euler(Variable dUdt, int i, int j, int k, double dt)
{
    U[i][j][k] = U[i][j][k] + dt * dUdt;
}
```

The Conserved Variables - Operator Implementation

```
static inline Variable operator+(const Variable &a, const Variable &b)
{
    Variable v;
    v.r = a.r + b.r;
    v.ru = a.ru + b.ru;
    v.E = a.E + b.E;
    return v;
}
```

```
static inline Variable operator*(const Variable &a, double n)
{
    Variable v;
    v.r = a.r * n;
    v.ru = a.ru * n;
    v.E = a.E * n;
    return v;
}
```

Automating Operator Implementation

- ▶ script part of the build process that generates these functions in C++.

Automating Operator Implementation

- ▶ script part of the build process that generates these functions in C++.
- ▶ extend C++ with introspection.

Automating Operator Implementation

- ▶ script part of the build process that generates these functions in C++.
- ▶ extend C++ with introspection.
- ▶ create a new programming language.

The Conserved Variables - Automated Operators

```
static inline Variable operator+(const Variable &a, const Variable &b)
{
    Variable v;
    for (auto M : Variable) v.*M = a.*M + b.*M;
    return v;
}
```

```
static inline Variable operator*(const Variable &a, double n)
{
    Variable v;
    for (auto M : Variable) v.*M = a.*M * n;
    return v;
}
```


Sections

Problem

- ▶ The System of Equations
 - ▶ *The Conserved Variables*
 - ▶ The Flux Function
 - ▶ Extra Information for Riemann Solver
 - ▶ Source Terms
- ▶ The Initial Conditions
- ▶ Boundary Conditions

Method

- ▶ **Domain Discretization**
- ▶ Riemann Solver
- ▶ Order of Accuracy
- ▶ Methods for Source Terms

Domain Discretization - 3d Regular Grid

```
Variable U[NX] [NY] [NZ];
Variable Fx[NX+1] [NY] [NZ];
Variable Fy[NX] [NY+1] [NZ];
Variable Fz[NX] [NY] [NZ+1];

void update_variables(double dt)
{
    for (int i=0; i<NX; i++) {
        for (int j=0; i<NY; j++) {
            for (int k=0; i<NZ; k++) {

                U[i] [j] [k] -= dt * ((Fx[i+1] [j] [k] - Fx[i] [j] [k]) / dx +
                                       (Fy[i] [j+1] [k] - Fy[i] [j] [k]) / dy +
                                       (Fz[i] [j] [k+1] - Fz[i] [j] [k]) / dz);
            }
        }
    }
}
```

Domain Discretization - General

```
array_over_cells<Variable> U;  
array_over_faces<Variable> F;  
  
void update_variables(double dt)  
{  
    for (cell i: allcells()) {  
        for (face j: facesofcell(i)) {  
            U[i] -= dt * (j.area() / i.volume()) * F[j];  
        }  
    }  
}
```

Domain Discretisation - Choices

- ▶ Regular Grid vs Irregular Mesh

Domain Discretisation - Choices

- ▶ Regular Grid vs Irregular Mesh
- ▶ Adaptive Mesh implementations

Domain Discretisation - Choices

- ▶ Regular Grid vs Irregular Mesh
- ▶ Adaptive Mesh implementations
- ▶ Domain parallelization

Domain Discretisation - Choices

- ▶ Regular Grid vs Irregular Mesh
- ▶ Adaptive Mesh implementations
- ▶ Domain parallelization
- ▶ GPU or CPU

Sections

Problem

- ▶ The System of Equations
 - ▶ *The Conserved Variables*
 - ▶ **The Flux Function**
 - ▶ **Extra Information for Riemann Solver**
 - ▶ Source Terms
- ▶ The Initial Conditions
- ▶ Boundary Conditions

Method

- ▶ *Domain Discretization*
- ▶ Riemann Solver
- ▶ Order of Accuracy
- ▶ Methods for Source Terms

The Flux Function

```
void point_flux(Variable &F, Variable U, dir d)
{
    vector3 u = U.ru / U.r;
    double p = (GAMMA-1) * (U.E - 0.5*U.ru*u);

    F.r = U.ru * d;
    F.ru = U.ru * (u * d) + p * d;
    F.E = (U.E + p) * (u * d);
}
```

Sections

Problem

- ▶ The System of Equations
 - ▶ *The Conserved Variables*
 - ▶ *The Flux Function*
 - ▶ *Extra Information for Riemann Solver*
 - ▶ Source Terms
- ▶ The Initial Conditions
- ▶ Boundary Conditions

Method

- ▶ *Domain Discretization*
- ▶ **Riemann Solver**
- ▶ Order of Accuracy
- ▶ Methods for Source Terms

Riemann Solver - HLL Implementation

```
void calculate_flux(Variable &F, const Variable &lU, const Variable &rU, dir d)
{
    real sl, sr;

    speeds2(sl, sr, lU, rU, d);
    if (sl > 0) point_flux(F, lU, d);
    else if (sr < 0) point_flux(F, rU, d);
    else {
        Variable lF, rF;

        point_flux(lF, lU, d);
        point_flux(rF, rU, d);
        F = (sr*lF - sl*rF + sr*sl*(rU - lU))/(sr-sl);
    }
}
```

Sections

Problem

- ▶ The System of Equations
 - ▶ *The Conserved Variables*
 - ▶ *The Flux Function*
 - ▶ *Extra Information for Riemann Solver*
 - ▶ Source Terms
- ▶ The Initial Conditions
- ▶ Boundary Conditions

Method

- ▶ *Domain Discretization*
- ▶ *Riemann Solver*
- ▶ **Order of Accuracy**
- ▶ Methods for Source Terms

Second Order - Minmod

```
void interpolate(Variable &fU, face f, dir d, real pos)
{
    cell i = f.cell();
    Variable dU = 0.5*minmod(U[i+d]-U[i], U[i]-U[i-d]);
    if (f.d == d) fU = U[i] - dU;
    else fU = U[i] + dU;
}
```

Sections

Problem

- ▶ The System of Equations
 - ▶ *The Conserved Variables*
 - ▶ *The Flux Function*
 - ▶ *Extra Information for Riemann Solver*
 - ▶ Source Terms
- ▶ **The Initial Conditions**
- ▶ Boundary Conditions

Method

- ▶ *Domain Discretization*
- ▶ *Riemann Solver*
- ▶ *Order of Accuracy*
- ▶ Methods for Source Terms

Sections

Problem

- ▶ The System of Equations
 - ▶ *The Conserved Variables*
 - ▶ *The Flux Function*
 - ▶ *Extra Information for Riemann Solver*
 - ▶ Source Terms
- ▶ *The Initial Conditions*
- ▶ **Boundary Conditions**

Method

- ▶ *Domain Discretization*
- ▶ *Riemann Solver*
- ▶ *Order of Accuracy*
- ▶ Methods for Source Terms

Sections

Problem

- ▶ The System of Equations
 - ▶ *The Conserved Variables*
 - ▶ *The Flux Function*
 - ▶ *Extra Information for Riemann Solver*
 - ▶ **Source Terms**
- ▶ *The Initial Conditions*
- ▶ *Boundary Conditions*

Method

- ▶ *Domain Discretization*
- ▶ *Riemann Solver*
- ▶ *Order of Accuracy*
- ▶ **Methods for Source Terms**

Source Terms

- ▶ Every Source Term is different
- ▶ Even simple ones might require well balancing
- ▶ Intrusive implementations
- ▶ 'Aspect Oriented' style

Code Insertion

```
const vector grav(0, 0, GRAVITY);

alter start calculate_simultaneous_sources(cell c)
{
    S[c].m -= grav * U[c].rho;
    S[c].E += grav * U[c].m;
}
```

Finite Difference Method

- ▶ Don't use Riemann Solver or Finite-volume high order methods

Finite Difference Method

- ▶ Don't use Riemann Solver or Finite-volume high order methods
- ▶ Need to provide a finite difference divergence formula
- ▶ And compatible source term methods

Finite Difference Method

- ▶ Don't use Riemann Solver or Finite-volume high order methods
- ▶ Need to provide a finite difference divergence formula
- ▶ And compatible source term methods
- ▶ Or function for U_t for other hyperbolic equations

For the Scientist

- ▶ Scientist has new problem

For the Scientist

- ▶ Scientist has new problem
- ▶ Implements model and maybe system of equations

For the Scientist

- ▶ Scientist has new problem
- ▶ Implements model and maybe system of equations
- ▶ Lots of standard solvers and other features already available

For the Scientist

- ▶ Scientist has new problem
- ▶ Implements model and maybe system of equations
- ▶ Lots of standard solvers and other features already available
- ▶ Can easily try all of them to see which one works best

For the Applied Mathematician

- ▶ Applied Mathematician designs new solver

For the Applied Mathematician

- ▶ Applied Mathematician designs new solver
- ▶ Implements solver using the framework, maybe altering similar one

For the Applied Mathematician

- ▶ Applied Mathematician designs new solver
- ▶ Implements solver using the framework, maybe altering similar one
- ▶ Lots of standard systems of equations and test cases already available

For the Applied Mathematician

- ▶ Applied Mathematician designs new solver
- ▶ Implements solver using the framework, maybe altering similar one
- ▶ Lots of standard systems of equations and test cases already available
- ▶ New test cases easy to add

Conclusions

- ▶ Implement algorithms without adding dependencies

Conclusions

- ▶ Implement algorithms without adding dependencies
- ▶ Easy to swap between alternative algorithms

Conclusions

- ▶ Implement algorithms without adding dependencies
- ▶ Easy to swap between alternative algorithms
- ▶ Less programming required for a new problem

Conclusions

- ▶ Implement algorithms without adding dependencies
- ▶ Easy to swap between alternative algorithms
- ▶ Less programming required for a new problem
- ▶ Future proofing as much as we can

Availability

`http://bitbucket.org/clef/clef/`