# **Compressible Fluid**

# Dynamics

# Fluids: Almost Everything

- 99% of the visible matter in the Universe is in the form of fluids
- Most of the astrophysical systems we don't fully understand, it's the fluid dynamics tripping us up



#### M42 - Orion Nebula

Credit: NASA, ESA, M. Robberto (STScI/ESA) and the Hubble Space Telescope Orion Treasury Project Team <u>http://antwrp.gsfc.nasa.gov/apod/ap060119.html</u>

# Equations of Hydrodynamics

- Density, momentum, and energy equations
- Supplemented by an equation of state - pressure as a function of dens, energy

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{v}) = 0$$
$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p$$
$$(\rho E) + \nabla \cdot ((\rho E + p) \mathbf{v}) = 0$$

 $rac{\partial}{\partial t}$ 

# Discretizing Derivatives

- Done by finite differencing the discretized values
- Implicitly or explicitly involves interpolating data and taking derivative of the interpolant
- More accuracy larger 'stencils'

$$\left. \frac{d^2 Q}{dx^2} \right|_i \approx \frac{Q_{i+1} - 2Q_i + Q_{i-1}}{\Delta x^2}$$





# Discretizing Derivatives

- Explicit hydrodynamics: only need information from as far away as the stencil reaches
- Nearest few neighbors
- Locality galore!



# Guardcells

- How to deal with boundaries?
- Because stencil juts out, need information on cells beyond those you are updating
- Pad domain with 'guard cells' so that stencil works even for the 0th point in domain
- Fill guard cells with values such that the required boundary conditions are met

### Global Domain



ng = I loop from ng, N - 2 ng

# Guardcells

- Impose BCs before each timestep
- Our hydro code 3 common boundary conditions
- 'outflow', reflect, and periodic
- Outflow (-1)- cell 0 just gets value from 1
- Reflect (-2); mirror the values
- Periodic(-3); copy values from other side (cell 0 gets values from cell 6)





ng = I loop from ng, N - 2 ng

# Equations of Hydrodynamics

- Density, momentum, and energy equations
- Supplemented by an equation of state - pressure & temperature as a function of dens, energy

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{v}) = 0$$
$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p$$
$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot ((\rho E + p) \mathbf{v}) = 0$$

# Conservation Law form

- Conservation of mass, momentum, energy
- These are important properties, want numerical solver to maintain them

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}(\rho v_x) = 0$$

$$\int_{x_L}^{x_R} \frac{\partial}{\partial t}\rho dx = -\int_{x_L}^{x_R} \frac{\partial}{\partial x}(\rho v_x)$$

$$\frac{\partial}{\partial t} \text{Mass} = -(\rho v_x)_R + (\rho v_x)_L$$

Change in mass = -outflux + influx



## Finite Volume Method

- Conservative; very well suited to high-speed flows with shocks
- At each timestep, calculate fluxes using interpolation/finite differences, and update cell quantities.
- Use conserved variables -- eg, momentum, not velocity.



# Flux Calculations

- Compressible flows: common to use Godunov-based schemes
- At cell interfaces, a Riemann problem is solved -- exact solution to a fluid jump
- Expensive, but does a great job of dealing with shocks



# Flux Calculations

- We're using a 'central scheme' or 'Kurganov scheme'
- No Riemann solve; average over possible waves
- Averaging means shocks are smeared out compared to Riemann solvers; but much faster, simpler to code (particularly for RHD, MHD)



Del Zanna, Bucciantini (2002) A&A 390:1177

# Dimensional Splitting

- Strang Splitting: Operators (including X and Y hydro operators) can be done separately, at cost of limiting time accuracy to  $\Delta t^2$ .
- Not at all obvious that should work as well as it does.
- Makes code much easier get a I d solver working, build 3d solver trivially









# Hydrodynamics

- Finite volume dimensionally split central scheme
- Need only local info (+/- 2 zones in each dimension)
- Implemented with dimensional splitting; sweep in x, then y (then y, then x)





# Other Hydrodynamic approaches

- Finite difference approaches; don't work in fluxes. Easier to incorporate some types of physics with high time accuracy.
- Parallelization issues same as finite volume codes.



Richard Günther, University of Tübingen. <u>http://www.tat.physik.uni-tuebingen.de/~rguenth/</u>

# Other Hydrodynamic approaches

- Incompressible flows
- Additional complexity: elliptical solver (implicit scheme)
- What we have here + linear solvers
- Or Multigrid: also mostly guardcell filling



Mike Zingale, SUNY Stony Brook <u>http://www.astro.sunysb.edu/mzingale/pyro/</u>

# Other Hydrodynamic approaches

- SPH: no grid at all. Fluid parcels.
- Hard to do highly accurate schemes, but arguably better suited for some problems.
- Gadget-2
- Some of the same parallelization issues as N-body gravity



## Single-Processor hydro code

- cd hydro{c,f}; make
- ./hydro 100
- Takes options:
  - number of points to write
- Outputs image (ppm) of initial conditions, final state (plots density)
- display ics.ppm
- display dens.ppm





## Single-Processor hydro code

- Set initial conditions
- Loop, calling timestep() and maybe some output routines (plot() - contours)
- At beginning and end, save an image file with outputppm()
- All data stored in array *u*.

```
nx = n+4; /* two cells on either side for BCs */
ny = n+4;
u = alloc3d_float(ny,nx,NVARS);
initialconditions(u, nx, ny);
outputppm(u,nx,ny,NVARS,"ics.ppm",IDENS);
t=0.;
for (iter=0; iter < 6*nx; iter++) {
    timestep(u,nx,ny,&dt);
    t += 2*dt;
    if ((iter % 10) == 1) {
        printf("%4d dt = %f, t = %f\n", iter, dt, t);
        plot(u, nx, ny);
    }
}
outputppm(u,nx,ny,NVARS,"dens.ppm",IDENS);
closeplot();</pre>
```

#### hydro.c

## Single-Processor hydro code

- Set initial conditions
- Loop, calling timestep() and maybe some output routines (plot() - contours)
- At beginning and end, save an image file with outputppm()
- All data stored in array u.

```
! boundary condition zones on e
nx = n+2*nguard
ny = n+2*nguard
allocate(u(nvars,nx,ny))
call initialconditions(u)
call outputppm(u,'ics.ppm',idens)
call openplot(nx, ny)
t=0
timesteps: do iter=1,nx*6
    call timestep(u,dt)
    t = t + 2*dt
    if (mod(iter, 10) == 1) then
      print *, iter, 'dt = ', dt, ' t = ', t
      call showplot(u)
    endif
end do timesteps
call outputppm(u,'dens.ppm',idens)
```

deallocate(u)

### hydro.f90

# Plotting to screen

- plot.c, plot.f90
- Every 10 timesteps
- Find min, max of pressure, density
- Plot 5 contours of density (red) and pressure (green)
- pgplot library (old, but works).



# Plotting to file

- ppm.c, ppm.f90
- PPM format -- binary (w/ ascii header)
- Find min, max of density
- Calculate r,g,b values for scaled density (black = min, yellow = max)
- Write header, then data.



```
u[j][i][IDENS] = projdens;
u[j][i][IMOMX] = projvel*projdens;
u[j][i][IMOMY] = 0.;
u[j][i][IENER] = 0.5*(projdens*projvel*projvel)+
```

if (r < 0.1\*sqrt(nx\*nx\*1.+ny\*ny\*1.)) {</pre>

## Data structure

- u:3 dimensional array containing each variable in 2d space
- eg, u[j][i][IDENS]
- or u(idens, i, j)

### solver.c (initialconditions)

```
where (r < 0.1*sqrt(nx*nx*1.+ny*ny))
    u(idens,:,:) =projdens
    u(imomx,:,:) =projdens*projvel
    u(imomy,:,:) =0
    u(iener,:,:) =0.5*(projdens*projvel*projvel)+1./(
elsewhere
    u(idens,:,:) =backgrounddens
    u(imomx,:,:) =0.
    u(imomy,:,:) =0.
    u(iener,:,:) =1./((gamma-1.)*backgrounddens)
endwhere</pre>
```

solver.f90 (initial conditions)







# Timestep routine

- Apply boundary conditions
- X sweep, Y sweep
- Transpose entire domain , so Y sweep is just an X sweep
- (unusual approach! But has advantages. Like matrix multiply.)
- Note dt calculated each step (minimum across domain.)

```
pure subroutine timestep(u,dt)
    real, dimension(:,:,:), intent(INOUT) :: u
    real, intent(OUT) :: dt
```

```
real, dimension(nvars,size(u,2),size(u,3)) :: ut
```

```
dt=0.5*cfl(u)
! the x sweep
    call periodicBCs(u,'x')
    call xsweep(u,dt)
! the y sweeps
    call xytranspose(ut,u)
    call periodicBCs(ut,'x')
    call xsweep(ut,dt)
    call periodicBCs(ut,'x')
    call xsweep(ut,dt)
! 2nd x sweep
    call xytranspose(u,ut)
    call periodicBCs(u,'x')
    call xsweep(u,dt)
end subroutine timestep
```

```
timestep
solver.f90
```

# Timestep routine

- Apply boundary conditions
- X sweep, Y sweep
- Transpose entire domain , so Y sweep is just an X sweep
- (unusual approach! But has advantages. Like matrix multiply.)
- Note dt calculated each step (minimum across domain.)

```
/oid timestep(float ***u, const int nx, const int ny, flo
    float ***ut;
```

```
ut = alloc3d_float(ny, nx, NVARS);
*dt=0.5*cfl(u,nx,ny);
```

```
/* the x sweep */
```

```
periodicBCs(u,nx,ny,'x');
xsweep(u,nx,ny,*dt);
```

```
/* the y sweeps */
xytranspose(ut,u,nx,ny);
periodicBCs(ut,ny,nx,'x');
xsweep(ut,ny,nx,*dt);
periodicBCs(ut,ny,nx,'x');
xsweep(ut,ny,nx,*dt);
```

```
/* 2nd x sweep */
xytranspose(u,ut,ny,nx);
periodicBCs(u,nx,ny,'x');
xsweep(u,nx,ny,*dt);
```

```
free3d_float(ut,ny);
```

#### L

### timestep solver.c

## Xsweep routine

- Go through each x "pencil" of cells
- Do Id hydrodynamics routine on that pencil.

```
pure subroutine xsweep(u,dt)
implicit none
real, intent(INOUT), dimension(:,:,:) :: u
real, intent(IN) :: dt
integer :: j

do j=1,size(u,3)
   call tvd1d(u(:,:,j),dt)
enddo
end subroutine xsweep
```

```
xsweep
solver.f90
```

```
void xsweep(float ***u, const int nx, c
    int j;
    for (j=0; j<ny; j++) {
        tvd1d(u[j],nx,dt);
    }
}</pre>
```

xsweep solver.c What do data dependancies look like for this?

# Data dependencies

- Previous timestep must be completed before next one started.
- Within each timestep,
- Each tvdld "pencil" can be done independently
- All must be done before transpose, BCs



# Looks like OpenMP!

- OpenMP of this code is trivial
- Wrap j loop with omp parallel for
- Almost all of the physics is in this tvd1d routine.

```
pure subroutine xsweep(u,dt)
implicit none
real, intent(INOUT), dimension(:,:,:) :: u
real, intent(IN) :: dt
integer :: j

do j=1,size(u,3)
    call tvd1d(u(:,:,j),dt)
enddo
end subroutine xsweep
```

```
xsweep
solver.f90
```

```
void xsweep(float ***u, const int nx, c
    int j;
    for (j=0; j<ny; j++) {
        tvd1d(u[j],nx,dt);
    }
}</pre>
```

xsweep solver.c

```
void xsweep(float ****u, const int nx, const int ny, const float dt){
    int j;
    #pragma omp parallel for default(none) shared(u) private(j)
    for (j=0; j<ny; j++) {
        tvdld(u[j],nx,dt);
    }
}</pre>
```

```
$ export OMP_NUM_THREADS=1
$ time ./hydro 100
real 0m7.256s
user 0m7.222s
sys0m0.003s
$ export OMP_NUM_THREADS=8
$ time ./hydro 100
real 0m1.453s
user 0m11.540s
```

sys0m0.044s

5x speedup with I line of code! (all output removed)

```
void xsweep(float ***u, const int nx, const int ny, const float dt){
    int j;
    #pragma omp parallel for default(none) shared(u) private(j)
    for (j=0; j<ny; j++) {
        tvdld(u[j],nx,dt);
    }
}</pre>
```

```
$ export OMP_NUM_THREADS=1
$ time ./hydro 500
real 3m36.728s
user 3m36.680s
sys0m0.013s
$ export OMP_NUM_THREADS=8
$ time ./hydro 500
real 0m47.459s
user 6m18.849s
```

sys0m0.598s

5x speedup with 1 line of code! (all output removed)

cfl(), xytranspose() could usefully be parallelized.

# MPling the code

• Domain decomposition



# MPling the code

- Domain decomposition
- For simplicity, for now we'll just implement decomposition in one direction, but we will design for full 2d decomposition


# MPling the code

- Domain decomposition
- We can do as with diffusion and figure out out neighbours by hand, but MPI has a better way...



#### Create new communicator with new topology

 MPI\_Cart\_create

 (MPI\_Comm comm\_old, int ndims, int \*dims, int \*periods, int reorder, MPI\_Comm \*comm\_cart)



#### Create new communicator with new topology

 MPI\_Cart\_create ( integer comm\_old, integer ndims, integer [dims], logical [periods], integer reorder, integer comm\_cart, integer ierr )









#### Let's try starting to do this together

- In a new directory:
- add mpi\_init, \_finalize, comm\_size.
- mpi\_cart\_create
- rank on *new* communicator.
- neighbours
- Only do part of domain



#### Next

- File IO have each process write its own file so don't overwrite
- Coordinate min, max across processes for contours, images.
- Coordinate min in cfl routine.



# MPling the code

- Domain decomposition
- Lots of data ensures locality
- How are we going to handle getting non-local information across processors?



# Guardcells

- Works for parallel decomposition!
- Job I needs info on Job 2s 0th zone, Job 2 needs info on Job Is last zone
- Pad array with 'guardcells' and fill them with the info from the appropriate node by message passing or shared memory
- Hydro code: need guardcells 2 deep







# Guard cell fill

- When we're doing boundary conditions.
- Swap guardcells with neighbour.



I: u(:, nx:nx+ng, ng:ny-ng) → 2: u(:, I:ng, ng:ny-ng)

2: u(:, ng+l:2\*ng, ng:ny-ng)  $\rightarrow$  l: u(:, nx+ng+l:nx+2\*ng, ng:ny-ng)

(ny-2\*ng)\*ng values to swap

# Cute way for Periodic BCs

- Actually make the decomposed mesh periodic;
- Make the far ends of the mesh neighbors
- Don't know the difference between that and any other neighboring grid
- Cart\_create sets this up for us automatically upon request.



- No different in principle than diffusion
- Just more values
- And more variables: dens, ener, imomx....
- Simplest way: copy all the variables into an NVARS\* (ny-2\*ng)\*ng sized buffer



I: u(:, nx:nx+ng, ng:ny-ng) → 2: u(:, I:ng, ng:ny-ng)

2: u(:, ng+l:2\*ng, ng:ny-ng)  $\rightarrow$  l: u(:, nx+ng+l:nx+2\*ng, ng:ny-ng)

nvars\*(ny-2\*ng)\*ng values to swap

- No different in principle than diffusion
- Just more values
- And more variables: dens, ener, temp....
- Simplest way: copy all the variables into an NVARS\* (ny-2\*ng)\*ng sized buffer



- Even simpler way:
- Loop over values, sending each one, rather than copying into buffer.
- NVARS\*nguard\* (ny-2\*nguard) latency hit.
- Would completely dominate communications cost.



- Let's do this together
- solver.f90; copy periodicBCs to gcBufferBCs
- When do we call this in timestep?

- This approach is simple, but introduces extraneous copies
- Memory bandwidth is already a bottleneck for these codes
- It would be nice to just point at the start of the guardcell data and have MPI read it from there.



- Let me make one simplification for now; copy whole stripes
- This isn't necessary, but will make stuff simpler at first
- Only a cost of 2xNg<sup>2</sup> = 8 extra cells (small fraction of ~200-2000 that would normally be copied)





- Recall how 2d memory is laid out
- y-direction guardcells contiguous



• Can send in one go:



```
call MPI_Send(u(1,1,ny), nvars*nguard*ny, MPI_REAL, ...)
ierr = MPI_Send(&(u[ny][0][0]), nvars*nguard*ny, MPI_FLOAT, ...)
```

- Creating MPI Data types.
- MPI\_Type\_contiguous: simplest case. Lets you build a string of some other type.

```
MPI_Datatype ybctype;
ierr = MPI_Type_contiguous(nvals*nguard*(ny), MPI_REAL, &ybctype);
ierr = MPI_Type_commit(&ybctype);
MPI_Send(&(u[ny][0][0]), 1, ybctype, ....)
```

Count

ierr = MPI\_Type\_free(&ybctype);



OldType &NewType

- Creating MPI Data types.
- MPI\_Type\_contiguous: simplest case. Lets you build a string of some other type.

```
integer :: ybctype
call MPI_Type_contiguous(nvals*nguard*(ny), MPI_REAL, ybctype, ierr)
call MPI_Type_commit(ybctype, ierr)
MPI_Send(u(1,1,ny), 1, ybctype, ....)
call MPI Type free(ybctype, ierr)
```

Count



OldType NewType

- Recall how 2d memory is laid out
- x gcs or boundary values *not* contiguous
- How do we do something like this for the x-direction?









call MPI\_Type\_commit(xbctype, ierr)

call MPI\_Send(u(1,nx,1), 1, ybctype, ...)



- Check: total amount of data = blocklen\*count = ny\*ng\*nvars
- Skipped over stride\*count = nx\*ny\*nvars





- Hands-On: Implement X guardcell filling with types.
- Copy gcBufferBC to gcTypeBC, implement.
- For now, create/free type each cycle through; ideally, we'd create/free these once.



# In MPI, there's always more than one way..

- MPI\_Type\_create\_subarray; piece of a multi-dimensional array.
- *Much* more convenient for higher-dimensional arrays
- (Otherwise, need vectors of vectors of vectors...)



```
int MPI_Type_create_subarray(
    int ndims, int *array_of_sizes,
    int *array_of_subsizes,
    int *array_of_starts,
    int order,
    MPI_Datatype oldtype,
    MPI_Datatype &newtype);
```

```
call MPI_Type_create_subarray(
    integer ndims, [array_of_sizes],
    [array_of_subsizes],
    [array_of_starts],
    order, oldtype,
    newtype, ierr)
```

# MPI-IO

- Would like the new, parallel version to still be able to write out single output files.
- But at no point does a single processor have entire domain...



# Parallel I/O

- Each processor has to write its own piece of the domain..
- without overwriting the other.
- Easier if there is global coordination



## MPI-IO

• Uses MPI to coordinate reading/writing to single file

te commodore te commodore te commodore

ierr = MPI\_File\_open(MPI\_COMM\_WORLD,filename, MPI\_MODE\_WRONLY | MPI\_MODE\_APPEND , MPI\_INFO\_NULL, &file);

#### ...stuff...

ierr = MPI\_File\_close(&file);

• Coordination -- collective operations.

# PPM file format

- Simple file format
- Someone has to write a header, then each PE has to output only its 3-bytes pixels skipping everyone elses.

```
header -- ASCII characters
```

'P6', comments, height/width, max val

```
P6
# min = 1.000000e+00, max = 4.733462e+01
100 100
255
(rgb)(rgb)(rgb)...
(rgb)(rgb)(rgb)...
row by row triples of bytes: each
pixel = 3 bytes
```

# MPI-IO File View

- Each process has a view of the file that consists of only of the parts accessible to it.
- For writing, hopefully non-overlapping!
- Describing this how data is laid out in a file is very similar to describing how data is laid out in memory...



# MPI-IO File View

 int MPI\_File\_set\_view( MPI\_File fh, MPI\_Offset disp, MPI\_Datatype etype, MPI\_Datatype filetype, char \*datarep, MPI\_Info info)

/\* displacement in bytes from start \*/

/\* elementary type \*/

/\* file type; prob different for each proc \*/
/\* 'native' or 'internal' \*/

/\* MPI\_INFO\_NULL for today \*/



# MPI-IO File View

- int MPI\_File\_set\_view( MPI\_File fh, MPI\_Offset disp, MPI\_Datatype etype, MPI\_Datatype filetype, char \*datarep, MPI\_Info info)
- /\* displacement in bytes from start \*/
- /\* elementary type \*/
- /\* file type; prob different for each proc \*/
  /\* 'native' or 'internal' \*/
- /\* MPI\_INFO\_NULL \*/



### MPI-IO File Write

 int MPI\_File\_write\_all( MPI\_File fh, void \*buf, int count, MPI\_Datatype datatype, MPI\_Status \*status)

Writes (\_all: collectively) to part of file within view.
## Hands On

• Implement the ppm routines collectively using the subarray type.