Notes

Fire

- [Nguyen, Fedkiw, Jensen '02]
- Gaseous fuel/air mix (from a burner, or a hot piece of wood, or …) heats up
- When it reaches ignition temperature, starts to burn
  - "blue core" - see the actual flame front due to emission lines of excited hydrocarbons
- Gets really hot while burning - glows orange from blackbody radiation of smoke/soot
- Cools due to radiation, mixing
  - Left with regular smoke

Defining the flow

- Inside and outside blue core, regular incompressible flow with buoyancy
- But an interesting boundary condition at the flame front
  - Gaseous fuel and air chemically reacts to produce a different gas with a different density
  - Mass is conserved, so volume has to change
  - Gas instantly expands at the flame front
- And the flame front is moving too
  - At the speed of the flow plus the reaction speed

Interface speed

- Interface = flame front = blue core surface
- $D=V_f-S$ is the speed of the flame front
  - It moves with the fuel flow, and on top of that, moves according to reaction speed S
  - S is fixed for a given fuel mix
- We can track the flame front with a level set ϕ
- Level set moves by

$$\phi_t + D|\nabla\phi| = 0$$
$$\phi_t + u_{LS} \cdot \nabla\phi = 0$$

- Here u_{LS} is u_f-Sn

Numerical method

- For water we had to work hard to move interface accurately
- Here it's ok just to use semi-Lagrangian method (with reinitialization)
- Why?
  - We're not conserving volume of blue core - if reaction is a little too fast or slow, that's fine
  - Numerical error looks like mean curvature
  - Real physics actually says reaction speed varies with mean curvature!

Conservation of mass

- Mass per unit area entering flame front is $\rho_f(V_f-D)$ where
  - $V_f=u_f \cdot n$ is the normal component of fuel velocity
  - D is the (normal) speed of the interface
- Mass per unit area leaving flame front is $\rho_h(V_h-D)$ where
  - $V_h=u_h \cdot n$ is the normal component of hot gaseous products velocity
- Equating the two gives:

$$\rho_f\left(V_f - D\right) = \rho_h\left(V_h - D\right)$$

Velocity jump

- Plugging interface speed D into conservation of mass at the flame front gives:

$$\rho_f S = \rho_h\left(V_h - V_f + S\right)$$
$$\rho_h V_h = \rho_h V_f + \rho_f S - \rho_h S$$
$$V_h = V_f + \left(\frac{\rho_f}{\rho_h} - 1\right) S$$

Ghost velocities

- This is a "jump condition": how the normal component of velocity jumps when you go over the flame interface
- This lets us define a "ghost" velocity field that is continuous
  - When we want to get a reasonable value of u_h for semi-Lagrangian advection of hot gaseous products on the fuel side of the interface, or vice versa (and also for moving interface)
  - When we compute divergence of velocity field
- Simply take the velocity field, add/subtract $(\rho_f/\rho_h-1)Sn$

Conservation of momentum

- Momentum is also conserved at the interface
- Fuel momentum per unit area "entering" the interface is $\rho_f V_f (V_f - D) + p_f$
- Hot gaseous product momentum per unit area "leaving" the interface is
$$\rho_h V_h (V_h - D) + p_h$$
- Equating the two gives
$$\rho_f V_f (V_f - D) + p_f = \rho_h V_h (V_h - D) + p_h$$

Simplifying

- Make the equation look nicer by taking conservation of mass:
$$\rho_f (V_f - D) = \rho_h (V_h - D)$$
multiplying both sides by -D:
$$\rho_f (-D)(V_f - D) = \rho_h (-D)(V_h - D)$$
and adding to previous slide's equation:
$$\rho_f (V_f - D)^2 + p_f = \rho_h (V_h - D)^2 + p_h$$

Pressure jump

- This gives us jump in pressure from one side of the interface to the other
- By adding/subtracting the jump, we can get a reasonable continuous extension of pressure from one side to the other
  - For taking the gradient of p to make the flow incompressible after advection
- Note when we solve the Poisson equation density is NOT constant, and we have to incorporate jump in p (known) just like we use it in the pressure gradient

Temperature

- We don't want to get into complex (!) chemistry of combustion
- Instead just specify a time curve for the temperature
  - Temperature known at flame front ($T_{ignition}$)
  - Temperature of a chunk of hot gaseous product rises at a given rate to T_{max} after it's created
  - Then cools due to radiation

Temperature cont'd

- For small flames (e.g. candles) can model initial temperature rise by tracking time since reaction: $Y_t+u\cdot\nabla Y=1$ and making T a function of Y
- For large flames ignore rise, just start flame at T_{max} (since transition region is very thin, close to blue core)
- Radiative cooling afterwards:

$$T_t + u \cdot \nabla T = -c_T \left(\frac{T - T_{air}}{T_{\max} - T_{air}} \right)^4$$

Smoke concentration

- Can do the same as for temperature: initially make it a function of time Y since reaction (rising from zero)
  - And ignore this regime for large flames
- Then just advect without change, like before
- Note: both temperature and smoke concentration play back into velocity equation (buoyancy force)

Note on fuel

- We assumed fuel mix is magically being injected into scene
  - Just fine for e.g. gas burners
  - Reasonable for slow-burning stuff (like thick wood)
- What about fast-burning material?
  - Can specify another reaction speed S_{fuel} for how fast solid/liquid fuel turned into flammable gas (dependent on temperature)
  - Track level set of solid/liquid fuel just like we did the blue core

SPH

- Smoothed Particle Hydrodynamics
  - A particle system approach
- Get rid of the mesh altogether - figure out how to do ∇p etc. with just particles
- Each particle represents a blurry chunk of fluid
  (with a particular mass, momentum, etc.)
- Lagrangian: advection is going to be easy

Mesh-free?

- Mathematically, SPH and particle-only methods are independent of meshes
- Practically, need an acceleration structure to speed up finding neighbouring particles (to figure out forces)
- Most popular structure (for non-adaptive codes, i.e. where h=constant for all particles) is…
  a mesh (background grid)

SPH

- SPH can be interpreted as a particular way of choosing forces, so that you converge to solving Navier-Stokes
- [Lucy'77], [Gingold & Monaghan '77], [Monaghan…], [Morris, Fox, Zhu '97], …
- Similar to FEM, we go to a finite dimensional space of functions
  - Basis functions now based on particles instead of grid elements
  - Can take derivatives etc. by differentiating the real function from the finite-dimensional space

Kernel

- Need to define particle's influence in surrounding space (how we'll build the basis functions)
- Choose a kernel function W
  - Smoothed approximation to δ
  - W(x)=W(|x|) - radially symmetric
  - Integral is 1
  - W=0 far enough away - when |x|>2.5h for example
- Examples:
  - Truncated Gaussian
  - Splines (cubic, quartic, quintic, …)

Cubic kernel

- Use $W(x) = \frac{1}{h^3} f\left(\frac{|x|}{h}\right)$ where

$$f(s) = \frac{1}{\pi}\begin{cases} 1 - \frac{3}{2}s^2 + \frac{3}{4}s^3, & 0 \le s \le 1 \\ \frac{1}{4}(2-s)^3, & 1 \le s \le 2 \\ 0, & 2 \le s \end{cases}$$

  - Note: not good for viscosity (2nd derivatives involved - not very smooth)

Estimating quantities

- Say we want to estimate some flow variable q at a point in space x
- We'll take a mass and kernel weighted average
- Raw version: $Q(x) = \sum_j m_j q_j W\left(x - x_j\right)$
  - But this doesn't work, since sum of weights is nowhere close to 1
  - Could normalize by dividing by $\sum_j m_j W_j$ but that involves complicates derivatives…
  - Instead use estimate for normalization at each particle separately (some mass-weighted measure of overlap)

Smoothed Particle Estimate

- Take the "raw" mass estimate to get density: $\langle \rho(x) \rangle = \sum_j m_j W\left(x - x_j\right)$
  - [check dimensions]
- Evaluate this at particles, use that to approximately normalize:

$$\langle q(x) \rangle = \sum_j q_j \frac{m_j W\left(x - x_j\right)}{\rho_j}$$

Incompressible Free Surfaces

- Actually, I lied
  - That is, regular SPH uses the previous formulation
  - For doing incompressible flow with free surface, we have a problem
  - Density drop smoothly to 0 around surface
  - This would generate huge pressure gradient, compresses surface layer
- So instead, track density for each particle as a primary variable (as well as mass!)
  - Update it with continuity equation
  - Mass stays constant however - probably equal for all particles, along with radius

Continuity equation

- Recall the equation is $\rho_t + u \cdot \nabla \rho = -\rho \nabla \cdot u$
- We'll handle advection by moving particles around
- So we need to figure out right-hand side
- Divergence of velocity for one particle is $\nabla \cdot v = \nabla \cdot \left(v_j W\left(x - x_j\right)\right) = v_j \cdot \nabla W_j$
- Multiply by density, get SPH estimate:

$$\langle \rho \nabla \cdot v \rangle_i = \sum_j m_j v_j \cdot \nabla_i W_{ij}$$

Momentum equation

- Without viscosity: $u_t + u \cdot \nabla u = -\frac{1}{\rho}\nabla p + g$
- Handle advection by moving particles
- Acceleration due to gravity is trivial
- Left with pressure gradient
- Naïve approach - just take SPH estimate as before

$$\frac{dv_i}{dt} = \left\langle -\frac{1}{\rho}\nabla p \right\rangle = -\sum_j m_j \frac{p_j}{\rho_j^2} \nabla_i W_{ij}$$

Conservation of momentum

- Remember momentum equation really came out of F=ma (but we divided by density to get acceleration)
- Previous slide - momentum is not conserved
  - Forces between two particles is not equal and opposite
- We need to symmetrize this somehow

$$\frac{dv_i}{dt} = -\sum_j m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \nabla_i W_{ij}$$

  - [check symmetry - also note angular momentum]

SPH advection

- Simple approach: just move each particle according to its velocity
- More sophisticated: use some kind of SPH estimate of v
  - keep nearby particles moving together
- XSPH

$$\frac{dx_i}{dt} = v_i + \sum_j \frac{m_j \left(v_j - v_i \right)}{\frac{1}{2}\left(\rho_i + \rho_j \right)} W_{ij}$$

Equation of state

- Some debate - maybe need a somewhat different equation of state if free-surface involved
- E.g. [Monaghan'94]

$$p = B\left(\left(\frac{\rho}{\rho_0} \right)^7 - 1 \right)$$

- For small variations, looks like gradient is the same [linearize]
  - But SPH doesn't estimate -1 exactly, so you do get different results…

The End

- But my lifetime guarantee: you can ask me questions anytime about numerical physics stuff…