DNS and LES of Turbulence

J.B. McLaughlin

Definitions

- Direct Numerical Simulation (DNS): solution of the continuity and Navier-Stokes equation without modeling.
- Large Eddy Simulation (LES): approximate solution of the continuity and Navier-Stokes equation on a “coarse grid” with some modeling.

Numerical Solution of PDE's

- The solutions are computed at a discrete set of times with a "time step". This is called "time discretization".
- The dependent variables are computed on "grid points" that are separated by a "grid space". This is called "spatial discretization."

Example: Unsteady Thermal Conduction

- Governing equation:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

where α is the thermal diffusivity

Time Discretization

$$\frac{\partial T}{\partial t} = \frac{T(x, t_{n+1}) - T(x, t_n)}{\Delta t}$$

$$T(x, t_{n+1}) = T(x, t_n) + (\alpha \Delta t) \frac{\partial^2 T}{\partial x^2}$$

Low Order Explicit Methods

Euler forward

$$\frac{\partial^2 T}{\partial x^2} = \left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_n} + O(\Delta t)$$

Adams - Bashforth

$$\frac{\partial^2 T}{\partial x^2} = \frac{3}{2}\left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_n} - \frac{1}{2}\left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_{n-1}} + O(\Delta t^2)$$

Low Order Implicit Methods

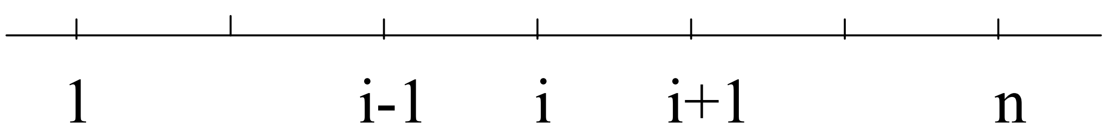
Euler backward

$$\frac{\partial^2 T}{\partial x^2} = \left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_{n+1}} + O(\Delta t)$$

Crank - Nicolson

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{2}\left(\left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_{n+1}} + \left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_n}\right) + O(\Delta t^2)$$

Spatial Discretization: 1D Uniform Grid.



Central Difference Approximation

$$\frac{\partial T}{\partial x} = \frac{T_{i+1} - T_{i-1}}{2\Delta x} + O(\Delta x^2)$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1} + T_{i-1} - 2T_i}{\Delta x^2} + O(\Delta x^2)$$

Discretized Equation

$$T_i^{n+1} = T_i^n + \left(\frac{\alpha \Delta t}{\Delta x^2}\right)\left(T_{i+1}^{n+1} + T_{i-1}^{n+1} - 2T_i^{n+1}\right)$$

"Tridiagonal" system of linear algebraic equations subject to boundary conditions at i=1 and i=N. Solve with Thomas algorithm.

Numerical Stability

The tridiagonal system is implicit so it is stable for all values of the time step and grid spacing. The only restriction is accuracy.

Fluid Mechanics

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p / \rho + \upsilon \nabla^2 \mathbf{u}$$

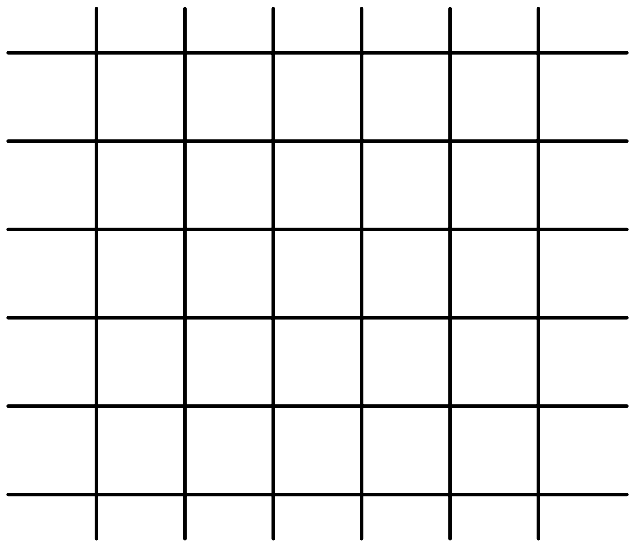
$$\nabla \cdot \mathbf{u} = 0$$

Navier-Stokes and continuity equations.

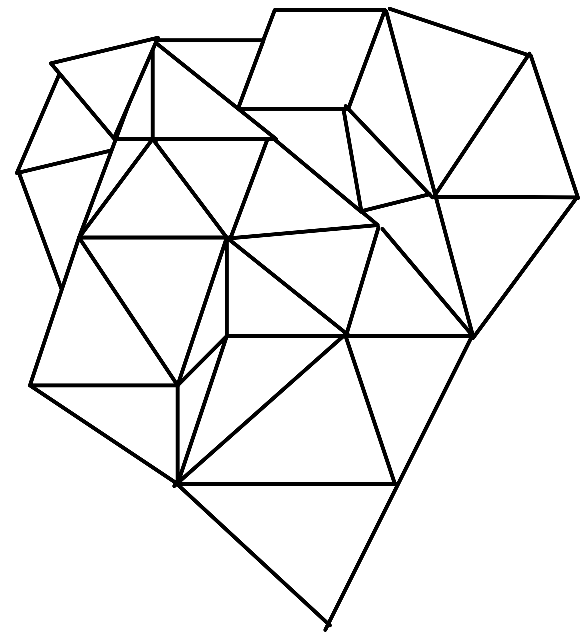
Time Discretization

The time discretization is the same as for the 1-D temperature equation.

Spatial Discretization (2D)



Structured grid



Unstructured grid

Structured Curvilinear Grid

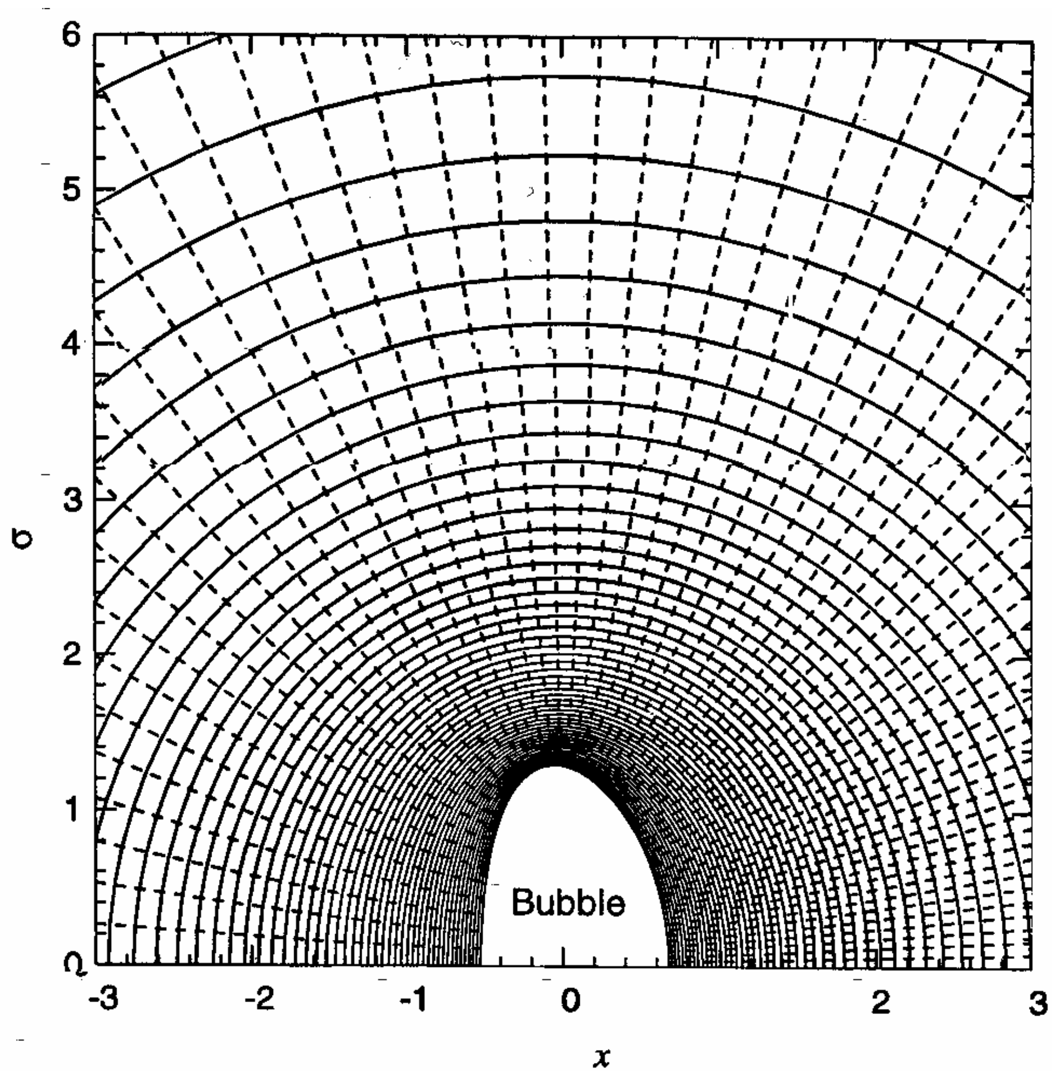


FIG. 1. Coordinate curves for a bubble with Re = 200, $W = 5$.

Structured Grids

- Each point can be labeled by a pair (2D) or a triplet (3D) of integers without ambiguity.
- Usually, structured grids are used with Cartesian or "body-fitted" curvilinear coordinate systems and the grid points lie on coordinate curves.

Unstructured Grids

- Unstructured grids are usually labeled with a global index for each “element” and a local coordinate for each grid point in the element.
- Typically, unstructured grids are used with finite element, boundary element, and spectral element methods and with “front-tracking” methods for 2 phase flow.

Fixed and Moving Grids

- Problems involving boundaries and interfaces that do not change with time are usually solved on fixed grids.
- Problems involving changing boundaries or interfaces (e.g., a spiraling bubble) can sometimes be done on a fixed grid, but it is often more convenient to use a moving grid.

Methods for Single Phase DNS

- Finite difference
- Finite volume
- Spectral
- Finite element (boundary element, spectral element)
- Lattice Boltzmann

Finite Difference Method (FDM)

- Easy to formulate discretized equations
- Algebraic convergence in space $O(h^p)$
- Useful for complex geometries if a body-fitted coordinate system can be found (axisymmetric geometry), otherwise "staircasing" and complex implementation of boundary conditions

Finite Volume Method (FVM)

- Based on more complicated integral formulation of governing equations than FDM.
- Conservation laws are satisfied exactly.
- Algebraic convergence.
- Useful for problems with body-fitted coordinate systems.

Spectral Method

- Easy to formulate discretized equations.
- Exponential spatial convergence (less resolution is needed than for FDM or others).
- Limited to very simple geometries (periodic box, channel flow between infinite flat walls).

Finite Element Method (FEM)

- More complicated mathematically than the other methods – based on variational formulation. Complicated matrices must be formed.
- Capable of handling extremely complicated, time-dependent geometries and two-phase flow.
- Algebraic convergence.

Lattice Boltzmann Method (LBM)

- New (1988) approach using kinetic equations for a “lattice gas”.
- Extremely simple to program.
- Parallelizes very efficiently.
- Abstract.
- Difficult to use grid refinement.
- Method is under development.

DNS of Two-Phase Flow

- Let us consider turbulent flows with solid or fluid particles in gases or liquids.
- For spherical particles that are smaller than the "Kolmogorov length", there are approximate equations of motion for the particles.
- In the "dilute" regime, small suspended particles have no "feedback" on the flow.

One-way Coupling Regime

- "One-way coupling" means that the suspended particles have no effect on the flow of the fluid.
- For aerosol particles, this condition may be expressed by requiring that the mass loading of the particles is very small compared to unity.

Aerosol Mass Loading

$$m_l = \phi \frac{\rho_p}{\rho_g} \qquad \frac{\rho_p}{\rho_g} = O(10^3)$$

where φ is the volume fraction,
ρ_p is the particle density,
ρ_g is the gas density.

Particle Equation of Motion for Small Spherical Particles

$$\frac{d\mathbf{v}}{dt} = \frac{\mathbf{F}}{m}$$

The force includes the drag, lift, gravitational, and Brownian forces.

Particle position vector

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}$$

$$\mathbf{r} = \mathrm{x}\mathbf{i} + \mathrm{y}\mathbf{j} + \mathrm{z}\mathbf{k}$$

Particle Tracking

- We solve Newton's law and the equation for the particle position vector as a set of 6 (in 3D) ODE's in time.
- Since the particles do not lie on grid points at any given time, it is necessary to use interpolation methods to compute the fluid velocity at the location of a particle.

Interpolation Methods

- Trilinear (simple, but introduces discontinuities at grid “cell” boundaries.)
- Legendre (more accurate, although discontinuities still exist).
- Hermite (complicated, but no discontinuities).

Next Class

- Spectral Method for DNS of turbulent flow in a periodic box.

- Tracking algorithm for small spherical particles in the above flow.