The Legacy and Future of CFD at Los Alamos

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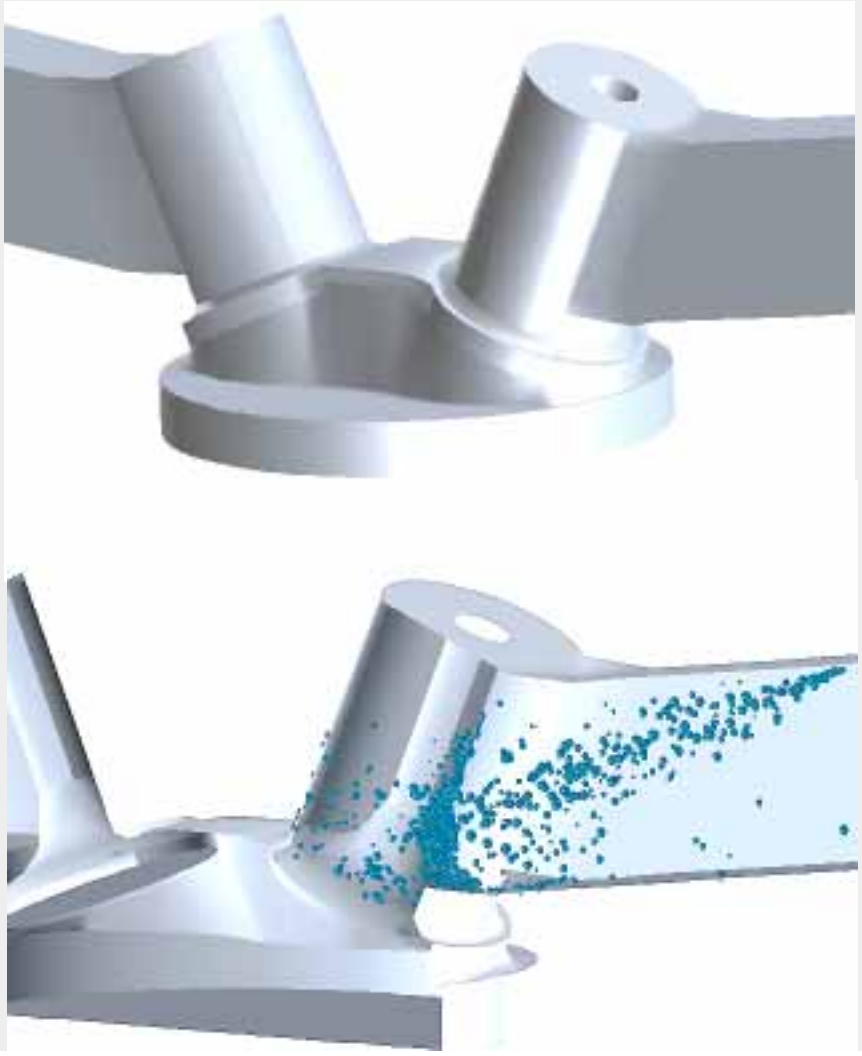
Reference: N. L. Johnson, LA-UR-96-1426,
Los Alamos National Laboratory, May 1996



Acknowledgments and Contacts

Early years
- Based on a lecture by Tony Hirt
- With Frank Harlow, Jerry Brackbill, John Dukowicz, Tony Amsden

Turbulence
- Tim Clark

Interface Tracking, Telluride, Pagosa, parallel computing
- Doug Kothe

Particle methods and FLIP
- Jerry Brackbill

CFDLIB and CCMAC
- Bryan Kashiwa and Brian VanderHeyden

Future of CFD
- Jerry Brackbill and John Dukowicz

And all the members of T-3, past and future

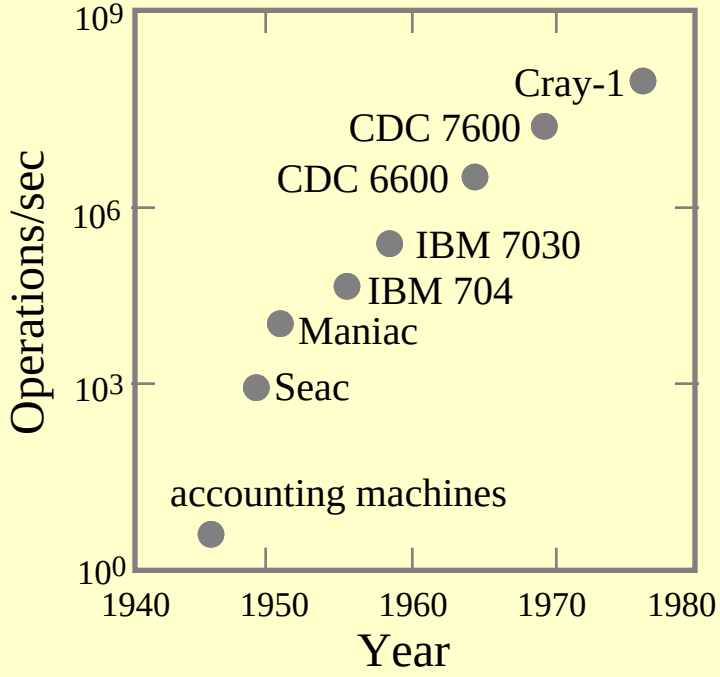
CDF at Los Alamos in 1956

Problems: Multiple materials under high compression, behaving like fluids, *with large flow distortion*.

Codes: Lagrangian with staggered variables.

Challenges: Mesh entanglement was fixed by hand.

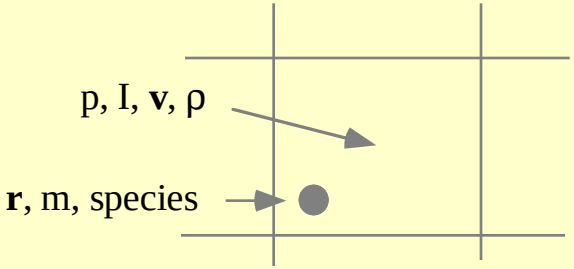
Computing resources: Maniac and IBM 704.



PIC - Solving the Unsolvable

Formulation:

Fixed Eulerian 2-D grid of equal size
Particles with species and mass



Treated:

Compressible flow
Multiple materials
Time dependent flow
Large distortion

First Use of Solution Phases:

Lagrangian -
Advance cell values without advection, map new values to particles.

Eulerian Advection -
Move particles.

Book Keeping -
Map particle information to mesh.
Partition energy in multi-material cells.

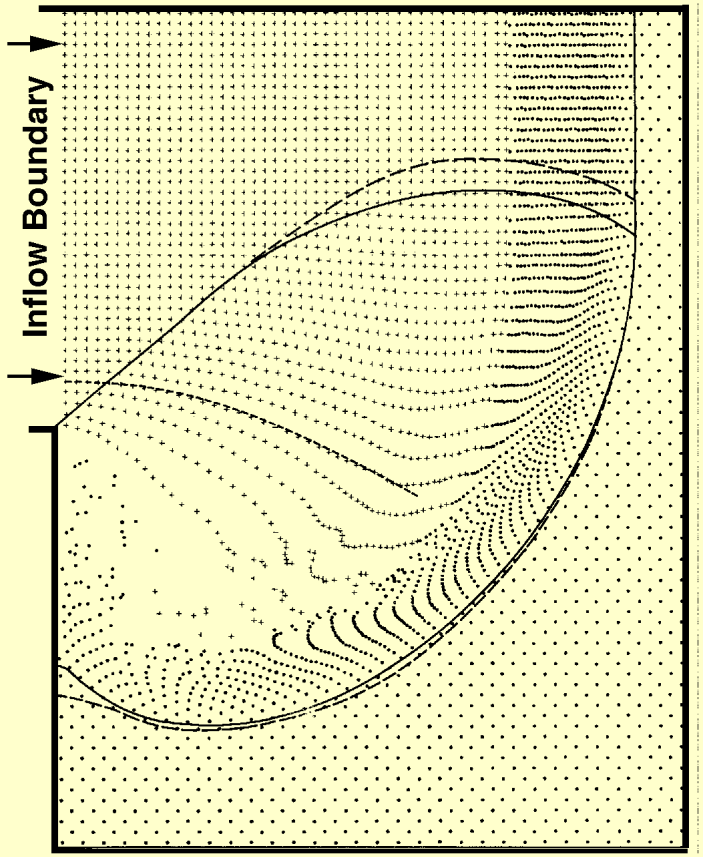
Comments:

First solutions of large deformations with distorting interfaces.

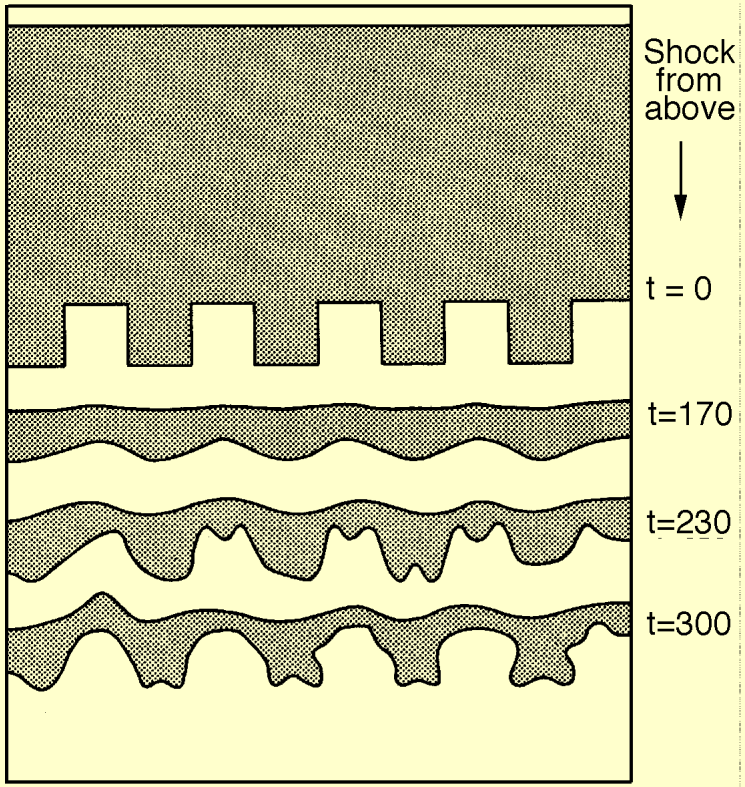
Problems with particle fluctuations -
16 particles per cell - minimum.

Should have been classified -
Large Particle method in Soviet Union,
Harlow, J. Ass. Comp. Mach. 4, 137 (1957).

PIC - Results



Shock compression of a single fluid:
Excellent comparison with experiments.
Particle resolution and stability.



Shock distortion with two materials:
Realistic interface instability.
Robust treatment of a difficult problem.

Vorticity-Stream Function Method (1963)

Problem: Solve 2-D, transient, *incompressible* flow.

Approach: Use non-primative variables to satisfy the incompressibility condition.

Comments:

Technique developed by Jacob Fromm with Frank Harlow,

Fromm and Harlow, Phys. Fluids 6, 975 (1963).

The solution to the von Karman vortex shedding problem made the cover of Scientific American.

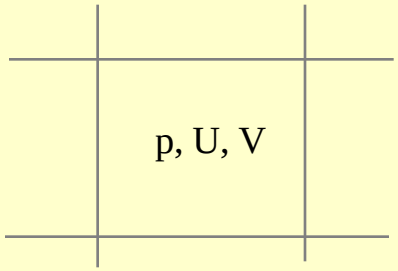
Later Fromm extended it to free-surface problems.

Fromm's *Phase Error Correction* method anticipated monotonicity preserving advection methods now so popular.

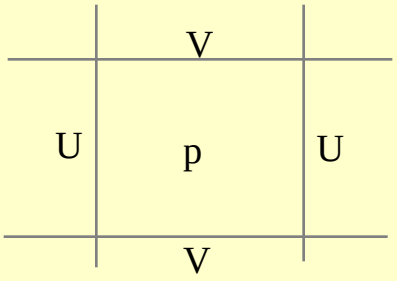
Origins of MAC: Marker and Cell Method

The MAC method (1965) was the origin of the "Staggered Mesh"

Cell Centered Mesh



Staggered Mesh



- "Checker board" pressure field.
- Difference approximations reach 2∂x.
- Now possible through nonlinear or temporal coupling.
- Single control volume.

- Coupled p-**v** fields.
- More compact support, ∂x.
- Simplified **v** boundary conditions.
- Multiple control volumes

Original MAC scheme used particles to "mark" the free surface.

Other T-3 CFD Methods

PAF (Particle and Force) in 1961 - Largely unknown method:

Goal: Eliminate the instabilities of mapping to the PIC Eulerian mesh.

Approach: Fluid represented by directly interacting mass points - Newtonian dynamics of many bodies with fluid-like forces.

- Suffered the same slowness and high memory costs of the PIC method.
- Exhibited extreme fluctuations as "fluid particles" reconnect.
- First of the Free-Lagrange method, precursor to SPH and Lattice-gas methods.

FLIC (Fluid in Cell) in 1966:

Goal: Eliminate particle fluctuations and high CPU costs associated with PIC.

Approach: Co-located state and kinetic variables at cell center; compute fluxes across cell boundaries.

- Exhibited classic instability from poorly couple pressure-momentum fields.
- First method to use Fractional Area/Volume formulation - never expolited.

k-ε Turbulence Model in 1967:

Goal: Introduce an additional length/time scale and dissipation equation.

- Used q-d because of the word processing at the time.

ICE (Implicit Continuous-Fluid Eulerian) in 1967, 1970:

Goal: Develop an all-speed algorithm - a generalized MAC method.

Origins of ALE: Arbitrary Lagrangian-Eulerian Method

First T-3 Lagrangian method (1967):

LINC (Lagrangian Incompressible)

Based on the cell volume remaining constant - not a zero-divergence.

Original formulation plagued by p-**v** null space oscillations.

Led to:

- Implicit p-**v** solution scheme, as later used for MAC.
- Showed necessity of automatic mesh rezoning (remapping).
- Explored elastic-plastic strength models and surface tension.

ALE capability was the second generation LINC development in 1974.

- The first finite-volume formulation.
- Precusor to the SALE and its progeny (Hirt) and FLIP (Brackbill).

Overview of the Early Days

The T-3 style:

- The focus was on the physics, not the mathematics.
- All techniques resulted from collaboration - no titles used.

The early days:

- Almost all territory was unexplored;
  every development found an application.
- Computing resourses were always a limiting factor.
- All graphing was done by hand (on Fridays).
- Each code was written from scratch.
- By 1966, 160 groups used the T-3 techniques
  and then use mushroomed.
- Codes were never distributed; SOLA was the first (1975).

Passing of an Era:

1968 was the last year that Harlow said he could keep up with all the CFD developments around the world.

Time Line of T-3 Activities

Computing Resources		Activities
Mechanical calculators	40's	All Lagrangian codes
Maniac	50's	Harlow and PIC arrive
IBM Stretch	60's	**T-3 established with 7 members** Vortex-stream function, PAF - Free Lagrangian
CDC 6600		MAC, ICE, k-ε turbulence LINC
CDC 7600 CRAY-1	70's	**Harlow steps down as Group Leader** MHD, ALE, Finite Volume Multiphase codes - SOLA
More CRAYs	80's	Reactive flows - RICE SALE Solid mechanics - ductile failure CAVEAT, Massively parallel codes
Clusters TMI CM-2 TMI CM-5 CRI T3D, Triton	90's	The return of Eulerian codes Grand challenges Fully unstructured codes **30 members**
????	2000	????

Current Research in T-3

Reactive Flow and Combustion
- Automotive flows
  - KIVA-3, KIVA-F90, KIVA-AC,
  - NO-UTOPIA,
  - Hydrogen-fueled powerplants
- Wildfire code for Crisis Management

Multiphase/Multimaterial/Multifield
- Reactive-multiphase flow (CFDLIB)
- High distortion flows (PAGOSA)
- Casting (TELLURIDE)

Particle methods
- MHD (FLIP)
- Granular flow modeling

Global modeling - Parallel computing
- Ocean flow modeling (POP)
- Ocean ice modeling (CICE)
- Coupled Ocean-Atmosphere modeling
- Mantle dynamics

Turbulence
- Spectral modeling
- Direct numerical simulations
- Engineering models

Material modeling
- High strain-rate plasticity
- Ductile and brittle failure
- Composites

Miscellaneous
- CO_2 elimination
- Underground tunnel location
- and others

Comments
- Mostly in collaboration
- Funding from
  - Industry partnerships
  - DOE thrust areas
  - Internal research support

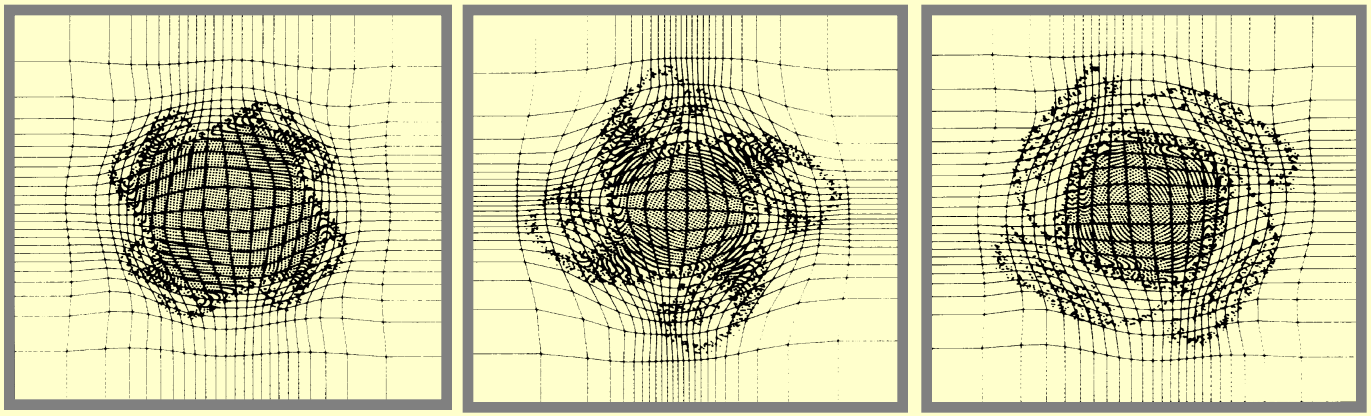
FLIP: A Modern PIC

Improvements over the historical PIC method:

- Mesh solution *updates* particle data
  - minimal numerical diffusion and finite-grid instability.
- Mesh is adaptive.
- Automatic particle density algorithm.
- Higher order interpolation to the mesh.
- Compact support for better mixed material treatment.
- Extension to 3-D, solid mechanics, plasmas, and MHD.

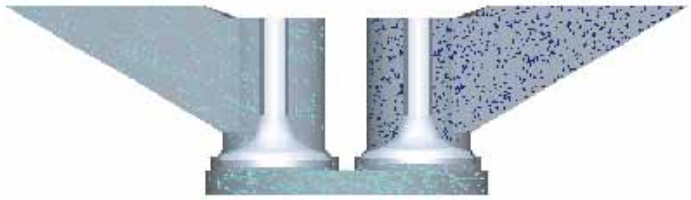
FLIP advantages over other non-particle methods:

- Galilean invariance for rotationally dominated flows.
- Lagrangian state storage for advection-challenged material models.

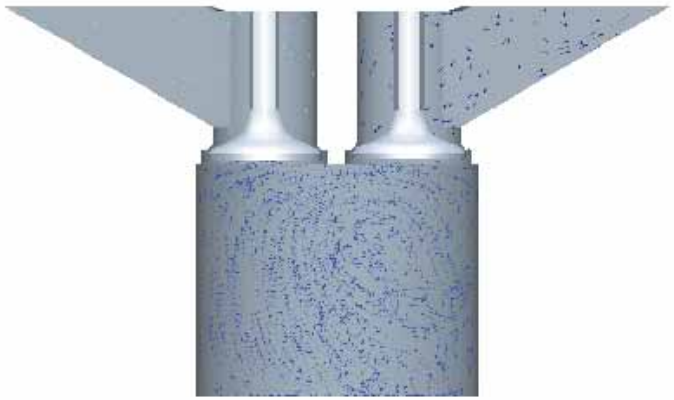


Solid rotation of a cylinder showing vorticity conservation, surface instabilities and mesh adaptivity.

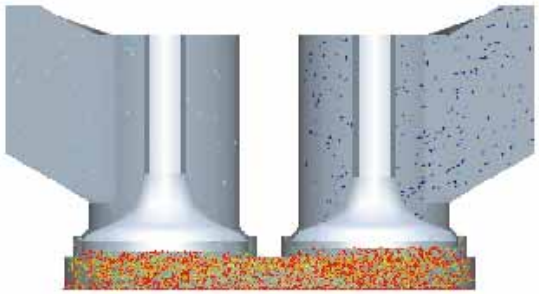
Hydrogen Combustion in the Onan Engine



Starting Conditions



Intake Flow



Combustion

Modeling of Discontinuities: Interfaces

The challenge:

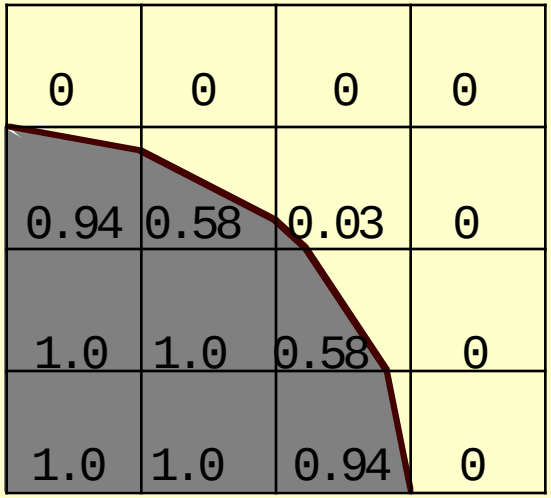
- Accuracy, efficiency and robustness in 3-D,
  not offered by PIC, VOF or interface tracking methods.

The approach:

1) Neglect sub-grid information.

2) Reconstruct interface (or discontinuity) each time step in 3-D,
based on grid information.

3) Use reconstruction to apply physics or for advection.



An example showing the reconstruction of a circle from volume fractions.

Comments:

- VOF origin, Youngs developed,
  extended to non-orthogonal meshes.
- Very powerful when combined with
  adaptive remapping as in CAVEAT.
- Major resurgence of Eulerian codes.
- Now basis of PAGOSA and TELLURIDE.

CFD Library and CCMAC

Origins: Late 1980's, development of a cell-centered ALE code - CAVEAT

- General purpose code for large distortional flows.
- Modular and efficient structure in 2-D and 3-D, using multi-block hexas.
- Resolved material interfaces *and* interface tracking with adaptivity.
- Explicit Godunov numerics with approximate Reimann solver
  - Difficult to implement additional physics.

Development of CCMAC: A cell-centered MAC scheme

- Uses TVD space-time centered fluxing method
  - Duplicates the staggered-grid p-**v** coupling.
  - Reduces to Lax-Wendroff scheme when space-time centered.
- Extended to all-speed flows
  - Requires a single Poisson pressure solutions each time step.
- Compatible with additional physics.

CFDLIB: A common library of CFD modules, based on CAVEAT

- All physics (compressible, incompressible, MHD, multiphase, ...)
- Reactive flows in heterogenous systems.
- Fluid-structure interactions

Turbulence Spectral Models

(T. Clarke and C. Zemach)

Consider a "Two-Point" Generalization of the Reynolds Stress Tensor (for a Single Fluid)

$$R_{ij}\left(\mathbf{x}_1,\mathbf{x}_2,t\right)=\left\langle u_i'\left(\mathbf{x}_1,t\right)u_j'\left(\mathbf{x}_2,t\right)\right\rangle$$

Derive an exact transport equation via Navier-Stokes and (1) change coordinates:

$$\mathbf{X}=\frac{1}{2}\left(\mathbf{x}_1+\mathbf{x}_2\right),\quad \mathbf{r}=\mathbf{x}_1-\mathbf{x}_2$$

(2) Fourier Transform with respect to the relative coordinate, **r** , and (3) perform angular integrations to reduce the vector-**k** space to a scalar k-space;

$$R_{ij}\left(\mathbf{x}_1,\mathbf{x}_2,t\right)\xrightarrow{1}R_{ij}\left(\mathbf{X},\mathbf{r},t\right)\xrightarrow{2}R_{ij}\left(\mathbf{X},\mathbf{k},t\right)\xrightarrow{3}R_{ij}\left(\mathbf{X},k,t\right)$$

Result: A spectral model of the turbulent Reynolds stress, related to the "single-point" engineering model by integration over wavenumber;

$$R_{ij}\left(\mathbf{X},t\right)=\int_0^\infty R_{ij}\left(\mathbf{X},k,t\right)dk=2\int_0^\infty E_{ij}\left(\mathbf{X},k,t\right)dk$$

where the "Energy Spectrum" $E(k,t)$ is $E_{nn}(k,t)$, the turbulent kinetic energy $K(t)$ is

$$K(\mathbf{X},t)=\int_0^\infty E(\mathbf{X},k,t)dk$$

- Requires no dissipation equation, or length-scale equation.
- Permits computation of "non-equilibrium" turbulence.
- Cost of direct numerical solution is much more costly than using a spectral model, which is more costly then using an engineering closure.

Turbulence and Symmetry

"A turbulent flow, initialized at t=0 in some arbitrary way, may relax, after some transient period, to a self-similar flow."

The turbulence *may* satisfy the same symmetries and scalings as the governing equations, i.e., the Navier-Stokes Equations.

Self-Similarity originates in invariance of the turbulence dynamics under a group of transformations, e.g., space-time transformations such as (for isotropic)

$$t' = \rho t, \qquad (time\ \ scaling),$$

$$t' = t + t_0 \qquad (time\ \ translation),$$

$$\mathfrak{l}' = \sigma \mathfrak{l} \qquad (length\ \ scaling).$$

Consider a scaling subgroup, $\rho^{\gamma} = \sigma$; for which an invariant solution obeys

$$\rho^{3\gamma-2} E(k,t) = E(\rho^{-\gamma} k, -t_0 + \rho(t + t_0)).$$

This can be shown to have a solution of the form (Karman-Howarth)

$$E(k,t) = K(t) L(t) f\left(kL(t)\right),$$

where $f(\xi)$ satisfies an auxiliary equation given by a theory, model, Navier-Stokes etc. Time dependencies are

$$K(t) = K_0 \,(1 + t/t_0)^{-\gamma_K}, \quad L(t) = L_0 (1 + t/t_0)^{\gamma},$$

and

$$\gamma_K = 2 - 2\gamma.$$

This agrees precisely with K-ε closures and with results from (all?) spectral models for isotropic turbulence.

Self-Similarity and Engineering Closures

Assertion: Single-Point (Engineering) closures can be rigorously correct in the limit of spectral self-similarity.

Consider the self-similar form for turbulence at high Reynolds number subjected to a *homogeneous mean* flow velocity gradient;

$$E_{ij}(k,t) = K(t)L(t)\,f_{ij}\big(kL(t)\big).$$

In general, each *fij* is different. During free decay, (upon releasing the mean flow strain or shear) the spectrum tends asymptotically towards the form

$$E(k,t) = K(t)L(t)\,f\big(kL(t)\big).$$

and

$$\tilde{E}_{ij}(k,t) = E_{ij}(k,t) - \frac{1}{3}\delta_{ij}E(k,t) = \tilde{K}_{ij}(t)L(t)\,\tilde{f}\big(kL(t)\big)$$

where

$$\tilde{K}_{ij}(t) = \frac{1}{2}\tilde{R}_{ij}(k,t) = \frac{1}{2}\left(R_{ij}(k,t) - \frac{1}{3}\delta_{ij}R_{nn}(k,t)\right)$$

Simple Group analysis (and the spectral model) predicts the same time dependencies of $\tilde{K}_{ij}(t)$ and $K(t)$. Hence the anisotropy, given by

$$b_{ij}(t) = \frac{\tilde{K}_{ij}(t)}{K(t)},$$

asymptotes to a constant--Hence, No Long-Term Return to Isotropy!

Conclusion: The detailed process of "Return Toward Isotropy" is a non-equilibrium process, not accurately depicted by engineering closures.

Example: Experiment of Uberoi & Wallis (J. Fluid Mech. **24**, 1979).

Lesson: One should not ask "too much" of an engineering closure.

Construction of Engineering Closures From Spectral Closures

(1) Determine the appropriate similarity group for the problem class.

-Might be an approximation.

-In conjunction with direct computation of the spectral model, and direct numerical simulation.

(2)Determine the self-similar form of the spectra.

(3) Substitute the self-similar expression into the spectral model equations, and take "appropriate" *k*-space moments.

"Appropriate" moments may be a product of the tastes of the researcher. E.G., does one want a dissipation rate equation or a length scale equation?

(4) Model coefficients will depend on spectral moments and are determined by the details of the self-similar forms produced by the spectral model.

Example: K-ε -b_{ij} models constructed from self-similar form for homogeneous mean-flow form.

K-Equation

$$\frac{\partial K(t)}{\partial t} = -2\frac{\partial U_n}{\partial x_m} b_{nm} - \varepsilon$$

where

$$b_{ij} = \int_0^\infty \tilde{f}_{ij}(\xi) d\xi .$$

ε-Equation

$$\frac{\partial \varepsilon}{\partial t} = -\left\{ g_{\varepsilon 0} b_{nm} + g_{\varepsilon 1} \phi_{nm} \right\} \frac{\partial U_m}{\partial X_n} \varepsilon - g_{\varepsilon 2} \frac{\varepsilon^2}{K}$$

where

$$g_{\varepsilon 0} = \frac{3m-2}{m},$$

$$g_{\varepsilon 1} = \left(\frac{3c_{F2}m+2}{m} \right),$$

$$g_{\varepsilon 2} = \frac{1}{m}\left(\frac{3m-2}{2} + \frac{1}{\alpha} \frac{J(m)}{I_{nn}(m)} \right),$$

$$\phi_{ij} = \frac{\tilde{I}_{ij}(m)}{I_{nn}(m)},$$

$$I_{ij}(m) = \int_0^\infty \xi^m f_{ij}(\xi) d\xi,$$

and

$$J(m) = \int_0^\infty \xi^m \frac{d}{d\xi} F_f(\xi) d\xi .$$

b_{ij}-Equation (Algebraic)

$$(c_B - 1)\left\{ \frac{\partial U_i}{\partial x_n} b_{nj} + \frac{\partial U_j}{\partial x_n} b_{ni} - \frac{2}{3}\delta_{ij} \frac{\partial U_m}{\partial x_n} b_{nm} \right\}$$

$$+ c_{B1}\left\{ \frac{\partial U_n}{\partial x_i} b_{nj} + \frac{\partial U_n}{\partial x_j} b_{ni} - \frac{2}{3}\delta_{ij} \frac{\partial U_m}{\partial x_n} b_{nm} \right\}$$

$$+ c_{B0}\left\{ \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right\} + 2\frac{\partial U_n}{\partial x_m} b_{nm} b_{ij}$$

$$= \frac{\varepsilon}{K}\left\{ \frac{c_M}{\alpha}\beta_{ij} - b_{ij} \right\},$$

where

$$\beta_{ij} = \int_0^\infty \xi^{3/2} f_{nn}^{1/2}(\xi)\, \tilde{f}_{ij}(\xi) d\xi .$$

Summary

Symmetry considerations and transformation groups within spectral turbulence models provide a framework to view the behavior of turbulence and closures without resort to ad-hoc modeling hypotheses.

Spectral models in simulations provide a much richer picture of the dynamics of turbulence and mix than do engineering closures, but at a greater computational cost.

In the limit of self-similarity (where a group transformation applies) engineering closures can be derived rigorously from spectral closures.

But, "equilibrium" engineering closure, in a *non-equilibrium* world, is at best, approximate.

Future Work

Focusing on the development of a rigorous nonhomogeneous theory that does not assume spectral scales are smaller than mean scales.

Examining 3-point spectral models to give guidance for closure techniques for 2-point models.

Derivation of multi-scale models or "reduced spectral" models for use in large computer codes;

- Applicable to non-self-similar turbulence.
- More tractable than full spectral closure.

Deferring effects of helicity ("swirl") until nonhomogeneous theory is developed.

Future of CFD

Current Status

- One method won't solve all problems.
- Distributed processing will be the largest computational resource.
- Grand Challenge problems still require supercomputers.
- Machine independence of codes has been *almost* achieved
  - Good software tools are more important than speed.
  - All new codes written in F90, with some C++.
  - Unstructured codes using *high-level* communication libraries.

Same problems now as in the beginning

- Efficiency, accuracy and robustness.
- Multi-scale phenomena.
- Treatment of nonlinear governing equations.
- Improvement of boundary conditions.
- Implementation of additional physics.

Areas of major future developments

- Operators based on fundamental properties of governing equations (conservation, symmetry, energy exchange, ...)
- Stochastic CFD codes
- Better methods for analysis of large data sets
- CFD code libraries - interchangeable methods and machines

Definitions of a CFD Code

I/O and boundary conditions are longer than the hydrodynamics.

Roubustness is often determined by an undocumented feature.

OR It is impossible to reconstruct a code from the manual.

Generates more information than can ever be studied, or even stored.

Capable of saturating all existing computing resources.

Great Lies of CFD Codes

"It will solve your problem without modifications."

"The manual has everything you need to run the code."

"Standardized graphics output, compatible with third party post-processors."

"Minimal learning curve."

"Executable on all machines with no modifications"

"Robust and accurate."

"All physics are compatible."

"User friendly."

"There are no more bugs in the code, only undocumented features."

"You can run the code without the manual."

"The technique was first developed here."