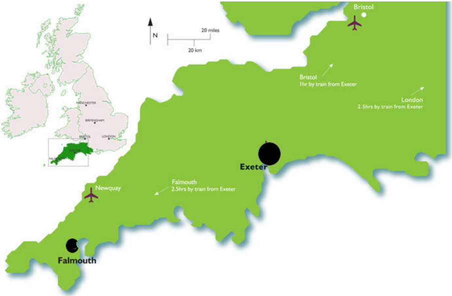
Computational Fluid Dynamics Research at the University of Exeter

Dr Gavin Tabor

CEMPS, University of Exeter

University of Exeter

- Founded 1922 – university status 1955
- "Top 10" non-specialist UK university



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CEMPS, CWS

College of Engineering. Maths and Physical Sciences

- One of 6 Colleges in University
- Formed from Schools of Physics, Engineering+Computer Science, CSM (Cornwall)
- Teaching and Research covering all aspects of Mathematical, Physical and Applied Sciences (Climate modelling, Renewable Energy, Materials, Biomechanics, Astrophysics...)

Several autonomous research groupings including the Centre for Water Systems

- Cross-disciplinary group in hydroinformatics and urban water systems
- Expertise includes hydraulics, systems analysis, EC, data mining ...

Research – GRT

CFD research in a number of areas :

- Basics of CFD – turbulence modelling, code development (OpenFOAM)
- Applications of CFD
  - Engineering applications – Urban Water Drainage, renewable energy
  - Biomedical applications – blood flow, air flow, Image Based Meshing

OpenFOAM

OpenFOAM is an Open Source CCM code/code library :

- Written in C++ – Based on FVM on arbitrary unstructured (polyhedral cell) meshes
- Originally developed by Henry Weller and others at IC (1990 – 2000); Nabla Ltd (2000 – 2004) as FOAM (Field Operation And Manipulation)
- Now released (2004 –) under Gnu GPL by OpenCFD Ltd. (http://www.opencfd.co.uk/)
- Fully featured – covers turbulent flow (LES,RANS), multiphase flow (Lagrangian, Eulerian, FSF), combustion, FSI, parallelisation . . .
- Extensive user community – Academic and commercial usage.

Strictly, OpenFOAM is not a CFD code – it is a C++ library of classes for writing CFD codes.

OpenFOAM uses the full range of the C++ language – inheritance, polymorphism, templating, operator overloading etc – where appropriate :

- Class mechanism – define new "types" for CFD
- Interface vs implementation : segregation of effort.
- Operator Overloading – provides standard mathematical syntax
- Inheritance, polymorphism etc – encodes relationships between conceptual entities in code

Effective result is a high level "language" for encoding CFD.

Advantages

Open Source software development encourages code sharing and information exchange. OpenFOAM's structure and use of C++ is ideal for this and provides a common platform for CFD research.

Advantages :

- Complete transparency and code availability (vs. "grey box" approach for commercial codes)
- Information exchange with other practitioners at a fundamental level
- CFD use not rationed by license fees.

Basic code designed to make implementing new models simpler (eg. overloading mathematical operators) and more rigorous (physical dimension checking)

Example : Burgers equation

1d Burgers equation :

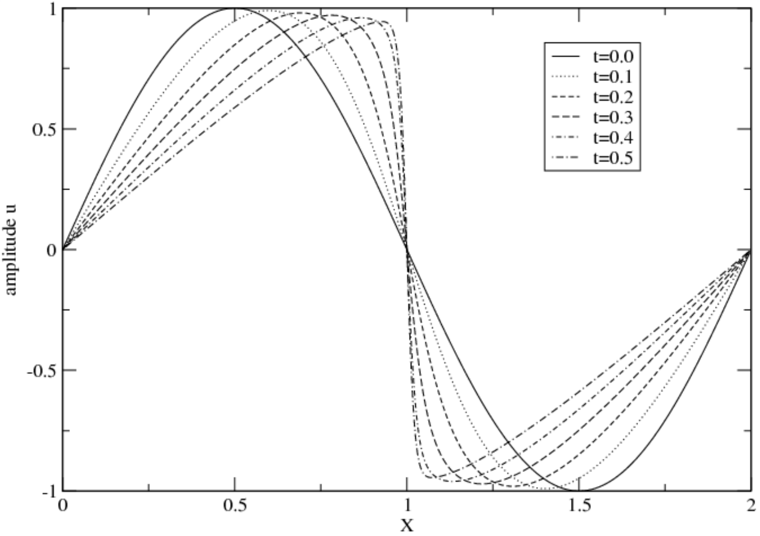
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$$

3d version (conservative form) :

$$\frac{\partial \underline{u}}{\partial t} + \nabla.(\frac{1}{2}\underline{u}\ \underline{u}) = \nu\nabla^2\underline{u}$$

```
fvVectorMatrix UEqn
(
    fvm::ddt(U)
  + 0.5*fvm::div(phi, U)
  - fvm::laplacian(nu, U)
);

UEqn.solve();
```



t=0.0
t=0.1
t=0.2
t=0.3
t=0.4
t=0.5
amplitude u
X
1
0.5
0
-0.5
-1
0
0.5
1
1.5
2

Outline of talk

1. Urban Drainage modelling (work within CWS) – Vortex Flow controls, flood runoff
2. Biomedical flow and Image Based Meshing
3. Microscale flow within porous media – packed beds and open-celled foams

Urban Drainage Modelling

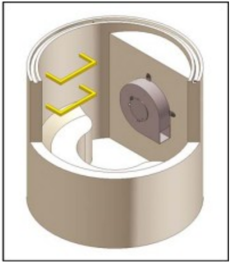
Two projects:

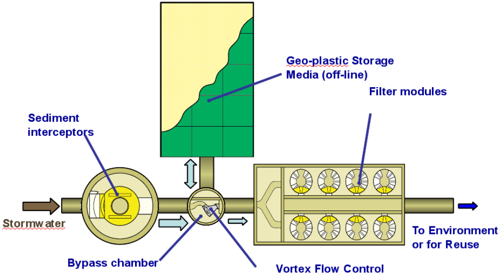
1. Vortex Flow Control
    - Industrial PhD project with UK company – Hydro International

2. Surface water runoff from road surface
    - Part of FRMRC-II project – large multi-centre research project in flood risk modelling

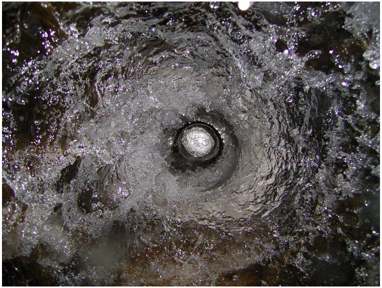
Vortex Flow Controls

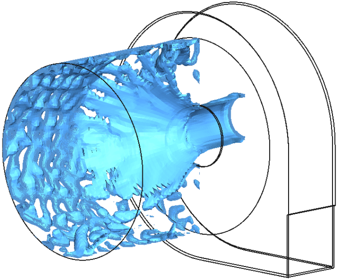
- KTP project with Hydro International
- VFC's used to switch stormwater flow to temporary storage





Vortex behaviour important – complex computational problem – free surface, turbulence modelling.





Examine surcharged and free-surface vortexing behaviour with CFD.

CFD

- Mesh refinement study – 100,000 to 4.5M cells
- Flow rates varied between $4l/s$ – $8l/s$
- Range of turbulence models used; $k - \epsilon$, $k - \omega$, DRSM
- Compared against experimental data (head loss, pressure tappings).
  - DRSM models give best results (turbulence significantly anisotropic)
  - EVM exhibit unphysical inflation of turbulent viscosity
- Transient behaviour important and captured through DRSM
- Both surcharged and free-discharge behaviour can be captured.

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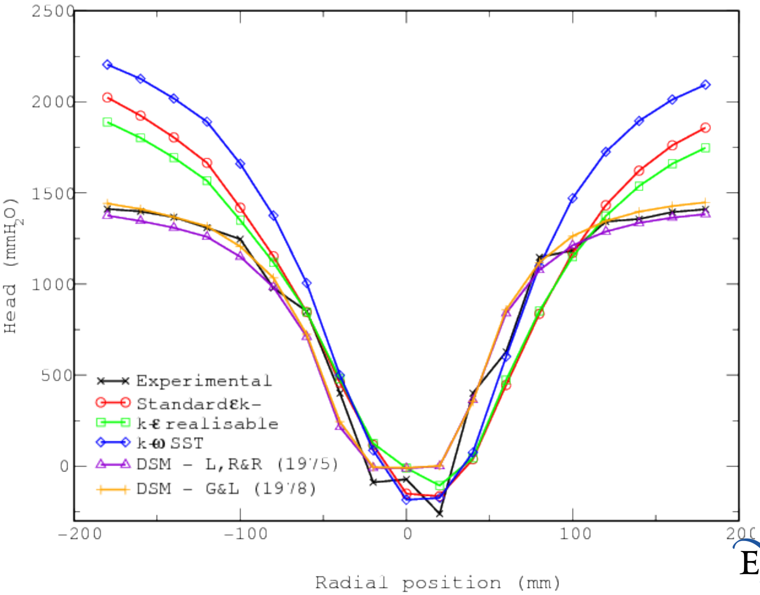
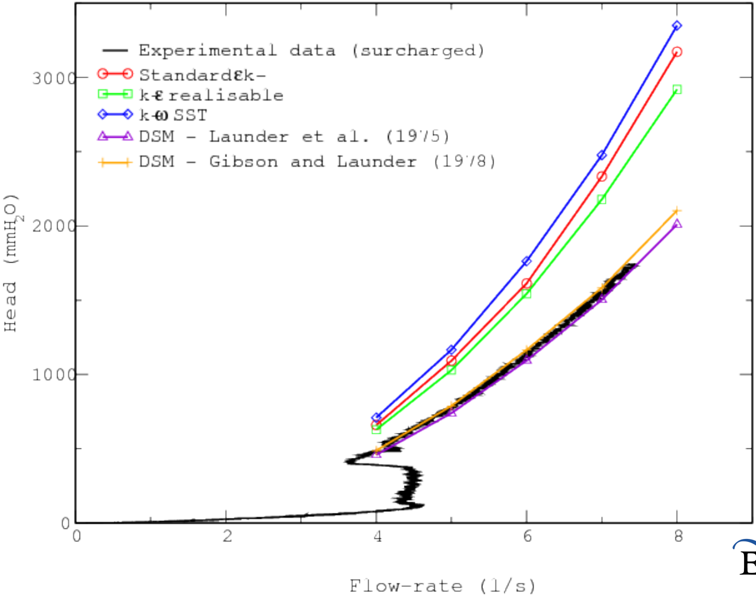
Pressure comparisons



Head loss



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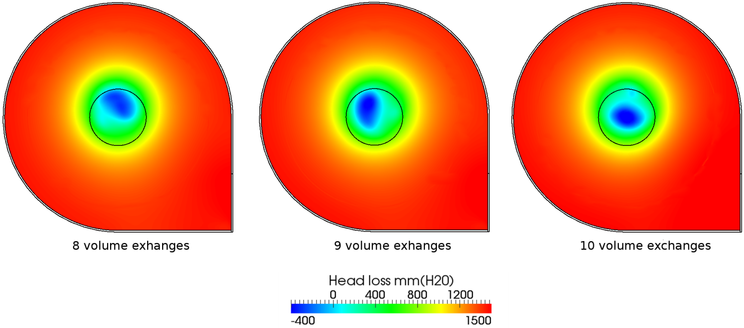
Pressure distribution

Flow instability present (vortex precession)



Summary

- Mesh refinement study – 100,000 to 4.5M cells
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Surface water runoff

Simulation of surface water runoff (FRMRC-II project) from roadway to gully pot.

- Critical point of coupling between 2d (surface flow) and 1d (pipe network) models
- Experimental data (Sheffield) to validate CFD models
- Vary all aspects of geometry + flow conditions
- Intention to develop empirical models for energy loss

CFD modelling

Problem must deal with both shallow depth effects and deep flow. Three approaches investigated :

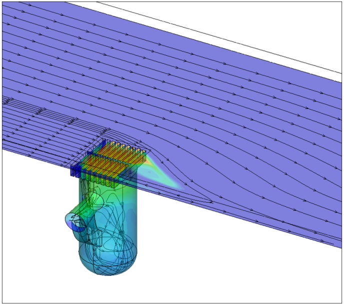
- Volume of Fluid method – indicator function taking values $[0, 1]$
- Investigating G-equation

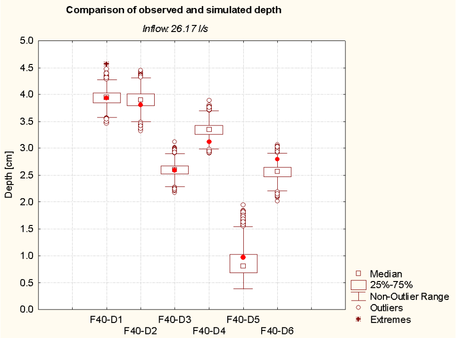
Problem; mesh resolution for thin surface flow makes mesh requirements prohibitive. Therefore:

- Finite Area approach (surface flow) coupled to VOF (gully pot).

Numerical details

- Solver: Implicit pressure based
- Multiphase model: Implicit VOF, level set
- Pressure velocity coupling: PISO
- Pressure discretization: PRESTO
- Turbulence closure: $k - \omega$ model
- Momentum discretization: 1st & 2nd order upwind
- Volume fraction discretization: 1st & 2nd order upwind




Comparison of observed and simulated depth
Inflow: 26.17 l/s
Depth [cm]
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
F40-D1
F40-D2
F40-D3
F40-D4
F40-D5
F40-D6
Median
25%-75%
Non-Outlier Range
Outliers
Extremes

Biofluid Mechanics

CCM – CFD, FE stress analysis – useful in biomedical field

- generate data that would be difficult to gather otherwise
- perform "experiments" that would be difficult (impossible, unethical) otherwise

Eg;

- CFD – blood flow in heart, arteries; air flow in lungs, trachea
- CSA – stress in bones, implants, impact analysis, soft tissue

Main problem – definition of geometry. Biomedical geometries

- complex over range of scales – possibly fractal
- patient-specific (individual differences possibly important)
- difficult to characterise mathematically
- ... and unknown – no blueprints available.

We need some way of determining the geometry. Various medical imaging techniques exist – MRI, CT etc.

Then need techniques to convert from image to mesh.

Image Based Meshing

IBM – automated methodology for generating geometry (+ mesh) from medical scans.

Many groups utilise 'CAD'-type approaches :

- create bounding geometry from stack of images
- then use existing automatic meshing techniques

e.g.

H. M. Ladak, J. S. Milner, and D. A. Steinman. ‘Rapid three-dimensional segmentation of the carotid bifurcation from serial mr images.’ *J. Biomech. Eng.*, 122(1):96 – 99, February 2000.

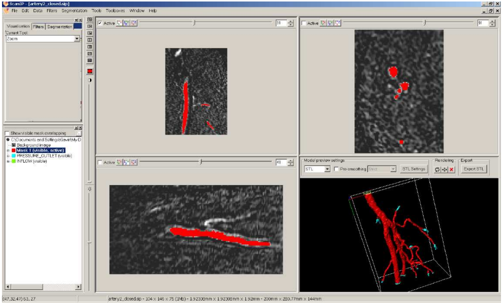
L. Antiga, B. Ene-Iordache, L. Caverni, G. P. Cornalba, and A. Remuzzi. ‘Geometric reconstruction for computational mesh generation of arterial bifurcations from ct angiography.’ *Computerized Medical Imaging and Graphics*, 26:227 – 235, 2002.

ScanIP/ScanFE

More direct approach to combine geometry detection and mesh creation – Voxel based methods.

ScanIP – Segments different volumes of interest from 3D data

- semi-automated and manual techniques
- includes various filters and thresholding tools



ScanFE

Base Cartesian mesh generated by marching cubes algorithm

- tetrahedronalised at boundaries based on cutting planes
- some adjustment to smooth boundary
- produces mixed tet/hex mesh
- adaptive meshing to reduce mesh density by agglomeration

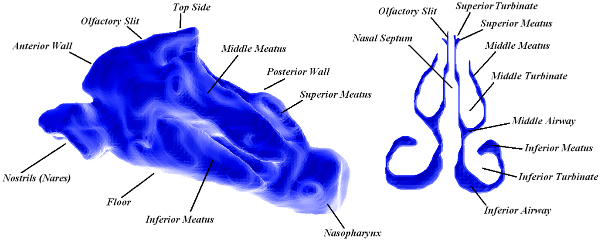
L. Zunarelli and P. G. Young. 'Analytical and numerical modelling of head injury mechanisms'. *Simulation and Modelling Techniques Applied to Medicine*, Institute of Physics, November 2-3, London, 1999.

Originally developed for FE stress analysis in bones – however FV CFD and FE techniques very similar (dual meshes).

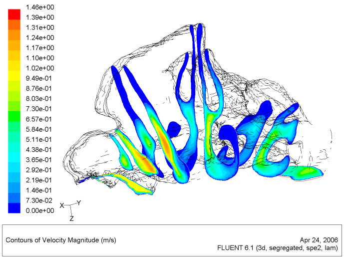
Develop FV output as cells and faces (Fluent mesh format) rather than points and edges (FEA).

Example – nasal air flow

Nasal geometry highly complex – nose acts to filter, humidify and warm air entering body.



Scan airways using MRI; segment using ScanIP; mesh using ScanFE. Calculations performed for constant inhalation (steady state) and single intake (transient). Compute air flow, temperature, relative humidity.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1.31e+00
1.24e+00
1.17e+00
1.10e+00
1.02e+00
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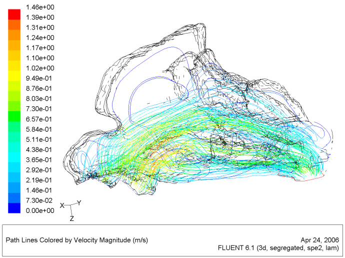
8.76e-01
8.03e-01
7.30e-01
6.57e-01
5.84e-01
5.11e-01
4.38e-01
3.65e-01
2.92e-01
2.19e-01
1.46e-01
7.30e-02
0.00e+00
X Y Z
Contours of Velocity Magnitude (m/s)
Apr 24, 2006
FLUENT 6.1 (3d, segregated, spe2, lam)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1.10e+00
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8.76e-01
8.03e-01
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6.57e-01
5.84e-01
5.11e-01
4.38e-01
3.65e-01
2.92e-01
2.19e-01
1.46e-01
7.30e-02
0.00e+00
X Y Z
Path Lines Colored by Velocity Magnitude (m/s)
Apr 24, 2006
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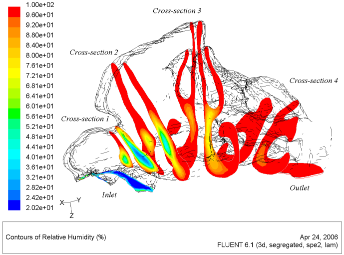
1.00e+02
9.60e+01
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8.80e+01
8.40e+01
8.00e+01
7.61e+01
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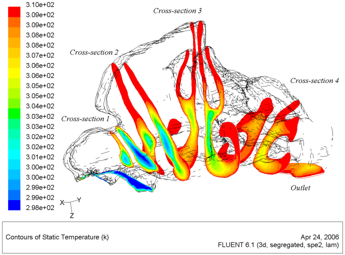
6.81e+01
6.41e+01
6.01e+01
5.61e+01
5.21e+01
4.81e+01
4.41e+01
4.01e+01
3.61e+01
3.21e+01
2.82e+01
2.42e+01
2.02e+01
Cross-section 3
Cross-section 2
Cross-section 4
Cross-section 1
Inlet
Outlet
X Y Z
Contours of Relative Humidity (%)
Apr 24, 2006
FLUENT 6.1 (3d, segregated, spe2, lam)


3.10e+02
3.09e+02
3.09e+02
3.08e+02
3.08e+02
3.07e+02
3.06e+02
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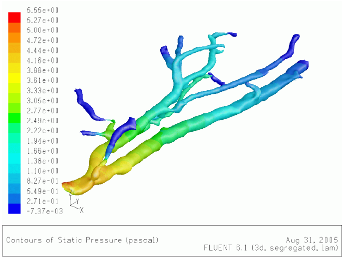
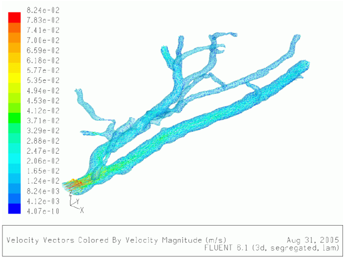
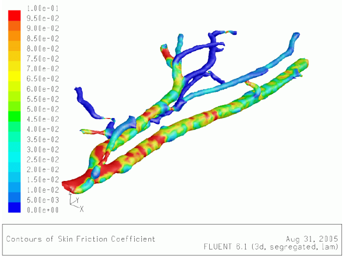
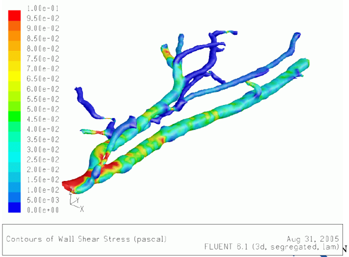
3.05e+02
3.05e+02
3.04e+02
3.03e+02
3.03e+02
3.02e+02
3.02e+02
3.01e+02
3.00e+02
3.00e+02
2.99e+02
2.99e+02
2.98e+02
Cross-section 3
Cross-section 2
Cross-section 4
Cross-section 1
Outlet
X Y Z
Contours of Static Temperature (k)
Apr 24, 2006
FLUENT 6.1 (3d, segregated, spe2, lam)

Blood flow – femoral artery









Packed Beds and Columns

Packed Bed – structure comprising a number of macroscopic particles packed into a particular volume

- Creates a network of space through which fluid can move
- Provides large surface area of contact between solid and fluid
- Particles can be random or uniform size/shape; structured/unstructured packing
- Valuable for heat exchange, combustion, catalysis, filtration etc.

Packed Column – packed bed enclosed within walls

Macroscopic flow properties determined by microstructural flow and geometry

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Empirical correlations

Most important: relation between flow speed and pressure drop – easilly measured experimentally.

Ergun equation (1950's) :

$$\frac{\Delta P}{L} = \frac{150\mu\left(1-\varepsilon\right)^2 U_S}{\varepsilon^3 d_P^2} + \frac{1.75\left(1-\varepsilon\right)\rho U_S^2}{\varepsilon^3 d_P}$$

Evaluation of coefficients and corrections for non-spherical particles determined experimentally. Eg. Eisfeld and Schnitzlein (2001) – compilation of 2300 experimental data points from 27 datasets.

Ergun equation limited to high aspect ratios : $(N = D/d_P) > 50$

Theoretical/computational analysis

Theoretical analysis – confined to simplified models eg. "bundle of straws" model, simplistic unit cells.

Computational analysis :

- Use CFD to probe microstructural flow
- Often restricted to simplified unit cells
- Lattice Boltzmann approach often used – increased speed, "voxelised" (non-body-fitted) geometry.

Challenges

Aim of project : to apply, validate and use FV CFD methods to compute flows through realistic bed geometries.

Challenges :

- **Geometry** Bed constructed and scanned (IBM) or synthesised using digital packing software (MacroPac)
- **Meshing** Resulting domains meshed using IBM or separate automatic mesh generation (Gambit)
- **Validation** Experimental measurements performed using equivalent or identical beds – eg using ALM to synthesise actual bed

Digital packing

Digital packing algorithms for packing objects (spheres) – eg. MacroPac – uses Monte Carlo methods to pack (includes simulated shaking).

Resulting output – list of sphere centres; imported into AutoCAD and used to reconstruct ACIS format for meshing.

Meshing strategies :

Gambit Import ACIS; use TGrid mesh generator and Tet/Hybrid options. TGrid uses wrapping technique to create triangular surface mesh; propagated into volume using Delauney triangulation.

IBM Create STL file for export to ScanFE via ScanCAD – alternative meshing strategy

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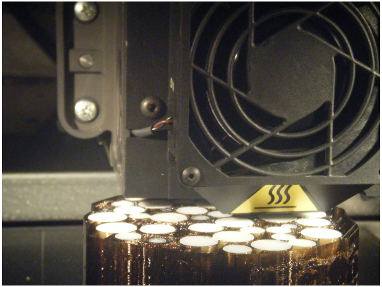
Experimentation

Parallel line of experiment – measure superficial velocity, pressure drop in air for equivalent beds.

Three approaches for making the bed :

- Use actual bed (when available)
- Manufacture equivalent bed eg. from marbles.
- Manufacture actual bed using ALM



Summary of cases investigated :

Model	Bed	Geometry	Meshing	Experiment
A	Spheres, diameter 14 mm	MacroPac	Gambit	Equivalent bed constructed of marbles
B	Cylinders, diameter 22 mm, length 30 mm	Physical packed bed	MRI Scan of bed + ScanFE	Physical packed bed
C	Spheres, diameter 16 mm	Physical packed bed	MRI scan of bed + ScanFE	Physical packed bed
D	Spheres, diameter 15 mm and 10 mm	MacroPac	ScanFE	Bed synthesised via RP

CFD

Computations carried out using Fluent

Unclear whether flow is turbulent or laminar;

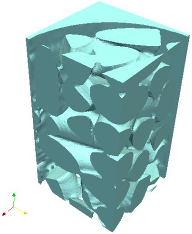
- Flow speeds cover range of $\mathcal{R}e$ – laminar to turbulent
- Mesh resolution fine – beyond Kolmogorov scale
- Distinction between laminar/transient and turbulent/steady state?

Calculations performed laminar, turbulent with $k - \omega$ and $k - \epsilon$ models; steady state (SIMPLE) and transient (PISO). Little difference between results.

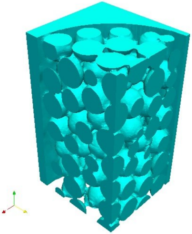
Geometry construction

Model B.

Model B.



Model C.

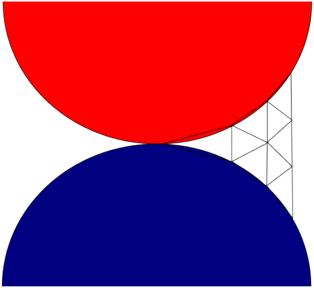


Mesh Construction

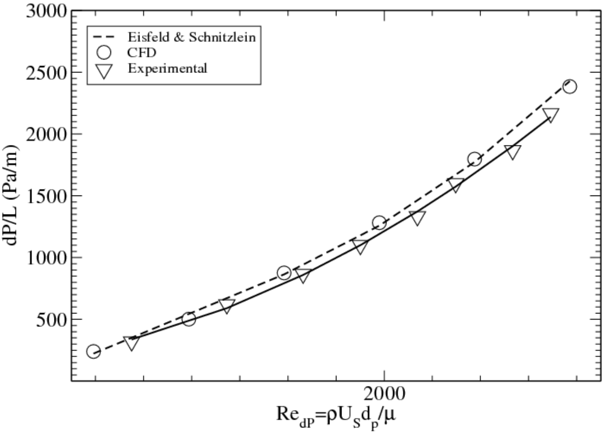
CAD-based meshing very challenging :

- Spheres meet at contact points – badly distorted cells
- Only small number of distorted cells; but dominate solution

IBM-based meshing broadens contact points – eliminates need for distorted cells. Flow in this region insignificant; no impact on solution accuracy.



Results – Model A



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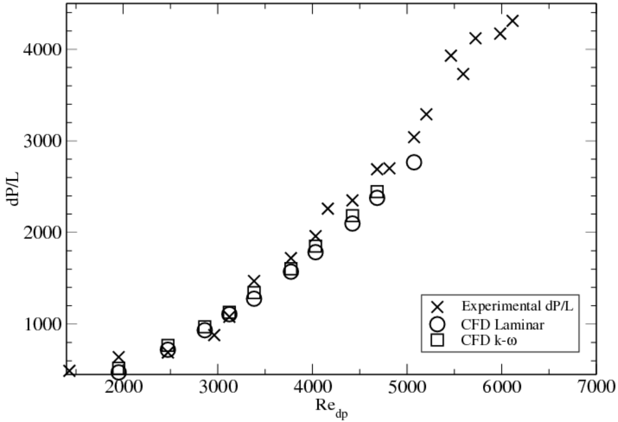
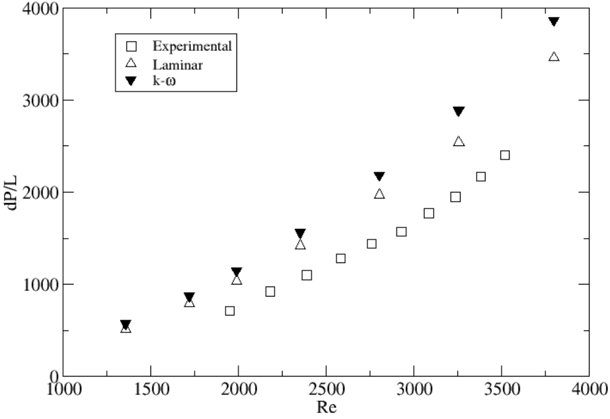
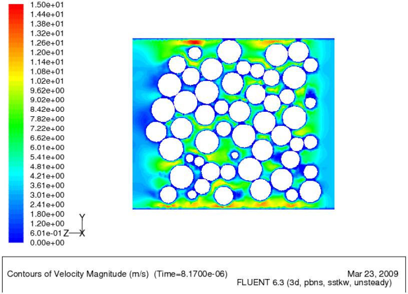
Results – Model B



Results – Model C



Velocities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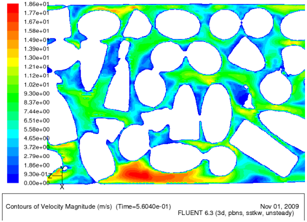
6.62e+00
6.01e+00
5.41e+00
4.81e+00
4.21e+00
3.61e+00
3.01e+00
2.41e+00
1.80e+00
1.20e+00
6.01e-01
0.00e+00
Y
Z
X
Contours of Velocity Magnitude (m/s) (Time=8.1700e-06)
Mar 23, 2009
FLUENT 6.3 (3d, pbns, sstkw, unsteady)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8.37e+00
7.44e+00
6.51e+00
5.58e+00
4.65e+00
3.72e+00
2.79e+00
1.86e+00
9.30e-01
0.00e+00
Contours of Velocity Magnitude (m/s) (Time=5.6040e-01)
Nov 01, 2009
FLUENT 6.3 (3d, pbns, sstkw, unsteady)

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Packed Beds Matt Baker

General Prof Hrvoje Jasak

Papers

"Computational fluid dynamics as a tool for urban drainage system analysis: A review of applications and best practice", D.S.Jarman, M.G.Faram, D.Butler, G.Tabor, V.R.Stovin, D.Burt, E.Throp. *11th International Conference on Urban Drainage, Edinburgh, Scotland* (2008)

"Comparison of LES of steady transitional flow in an idealised stenosed axisymmetric artery model with a RANS transitional model", F.P.P.Tan, N.B.Wood, G.Tabor, X.Y.Xu. To appear in :*J.Biomech.Engng* **133** (2011)

"Computational analysis of transitional air flow through packed columns of spheres using the finite volume technique", M.J.Baker, G. Tabor.*Computers and Chemical Engineering* **34** pp.878 – 885 (2010)

"OpenFOAM: An Exeter perspective", G.Tabor. *V.European Conference on Computational Fluid Dynamics* ECCOMAS CFD 2010, Lisbon,Portugal (2010)

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