An Overview of Computational Engineering at Daresbury

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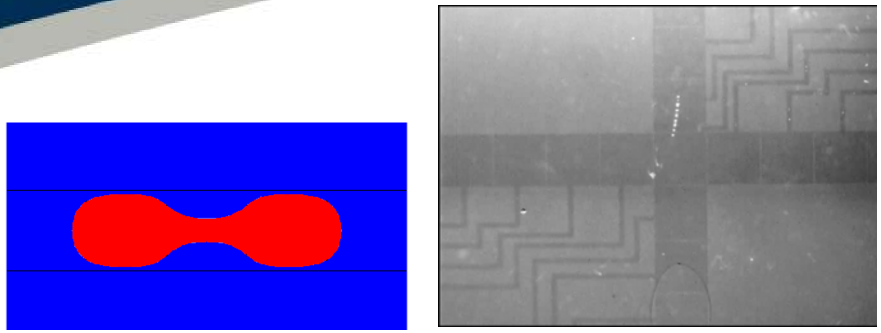
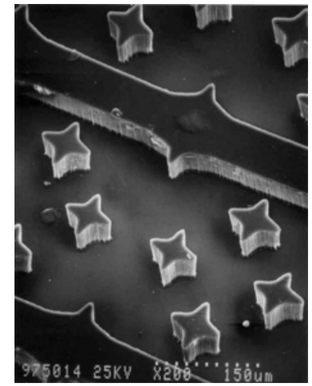
Computational Engineering Group

- The Computational Engineering Group at Daresbury Laboratory is part of SCD and focuses specifically on HPC capability to model a range of *fluid flows*
- The R&D activities cover a wide range of applications, including:
  - Turbulence and combustion
  - Free surface and capillary flows
  - Aerodynamics – mainly high speed
  - Environmental flow modelling
  - Microfluidics
  - Non-equilibrium/rarefied fluid phenomena

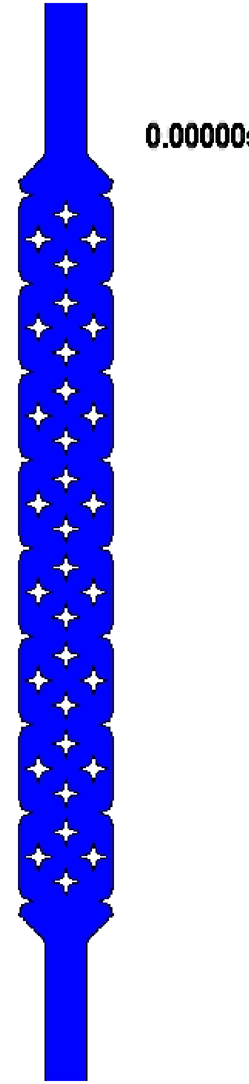
Example modelling activities



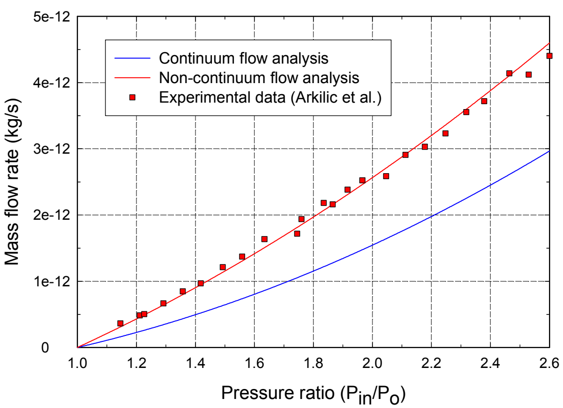
Modelling electrowetting-on-dielectric (EWOD) droplet handling for the MESA+ Institute of Nanotechnology, Univ. of Twente

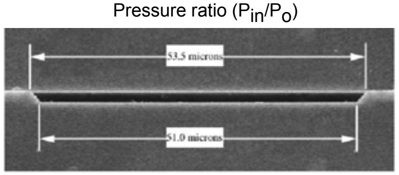


SEM image of micro-pillars

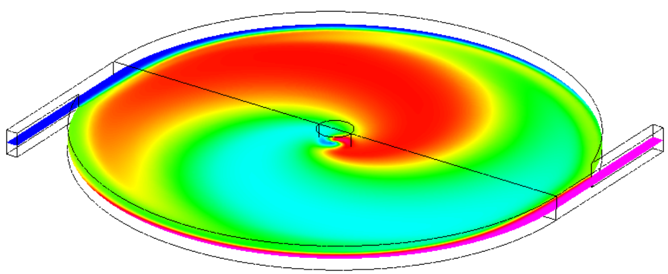


CFD modelling activities





Modelling gas flows in microfluidic devices



Simulation of a micro-vortex reactor for radiochemical synthesis with the Paterson Institute for Cancer Research

Simulation of a novel mixing element in a PCR reactor for CIGMR, Univ. of Manchester

Non-equilibrium/rarefied fluid phenomena

The conventional Navier-Stokes-Fourier (NSF) equations are the cornerstone of many fluid applications and leading-edge engineering designs.

They have been profoundly successful at capturing a diverse set of problems from transonic flow around an aircraft to creeping flow around a spherical particle.

However, there are cases when the NSF equations are a poor predictor of observed flow phenomena.

Discrepancies arise when the NSF equation are applied to problems where the fundamental assumptions behind these equations are breaking down.

This talk will focus on the challenge of finding computationally efficient ways to accurately and reliably capture the physics associated with non-equilibrium flow.

Validity of governing equations

Recall - the Navier-Stokes equations assume

The system is in thermodynamic equilibrium:

Martin Knudsen

Knudsen (15/2/1871) was a Danish physicist who worked on molecular gas flow (very low pressure). The Knudsen number is named after his pioneering work and is an indication of when the flow is in thermodynamic equilibrium.

$$Kn = \frac{\lambda}{L} = C\frac{M}{(Re)^n}$$

Here, λ is the *mean free path* and L is a suitable length scale.

For $Kn < 0.001$, the system is in thermodynamic equilibrium.

For $Kn \rightarrow \infty$, we have a *free molecular* regime. The Navier-Stokes equations are **NOT VALID**.

The Knudsen number Kn

$Kn = \lambda / L$

- Air at S.A.T.P: mean free path, $\lambda \sim 10^{-7}$ m
  device length $L \sim 10^{-6}$ m
- Hence $Kn \sim 0.1$
- Rarefaction effects can be appreciable

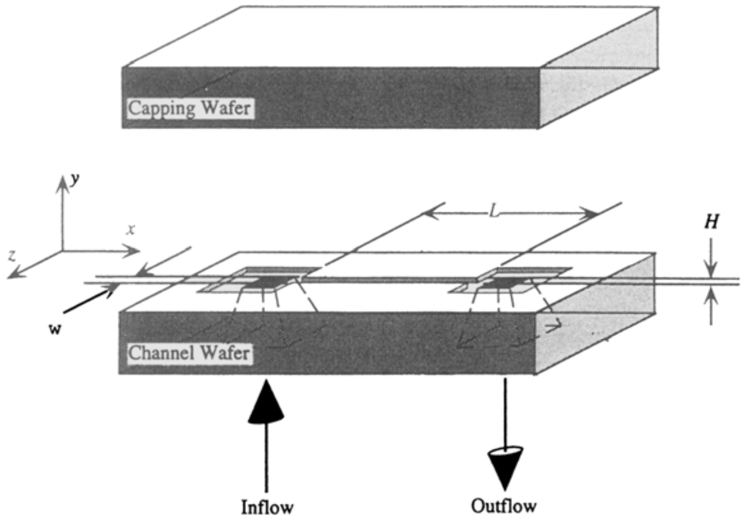
Euler	$Kn \to 0$
NSF	$Kn < 0.001$
NSF+slip	$0.001 \leq Kn \leq 0.1$
Transition	$0.1 \leq Kn \leq 10$
Free molecular	$Kn > 10$

What does this imply?

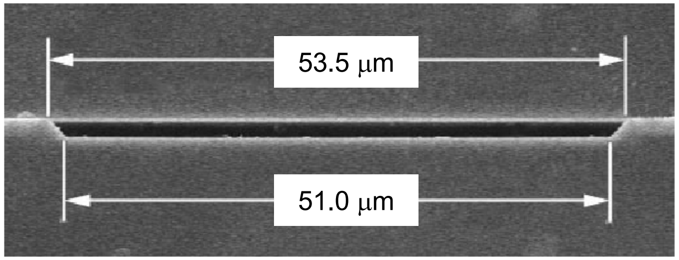
- Navier Stokes equations in conjunction with no-slip boundary conditions not valid for many gas flows in MEMS
- Slip-flow & temperature jump boundary conditions are needed
- All hydrodynamic quantities are affected e.g. mass flow rates, velocity gradients, wall shear stresses, drag forces……

Examples of the NSF equations breaking down

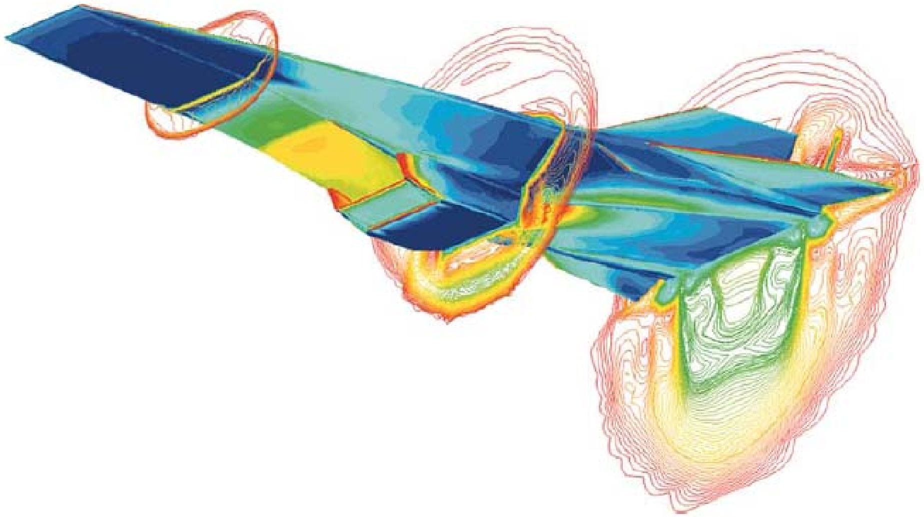
Consider two very different applications



Schematic view of silicon micro-machined channel (Arkilic *et al*., 1997)

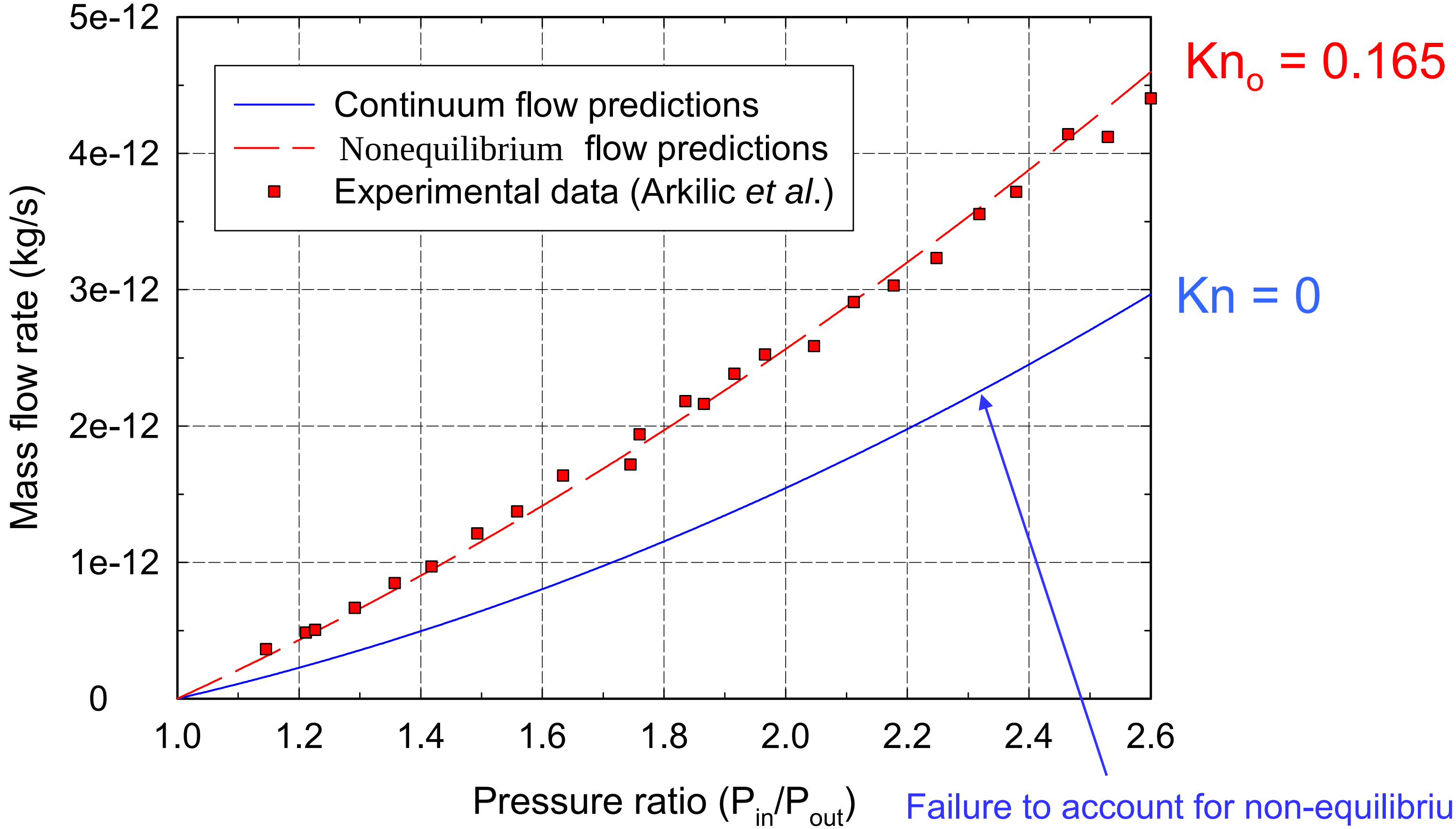


SEM of channel cross section: M ~ 0.0001



CFD prediction of Hyper-X flow field at M = 7 with engine operating. (Courtesy of NASA Dryden Flight Research Center).

Microfluidics: He mass flow rates through silicon channel

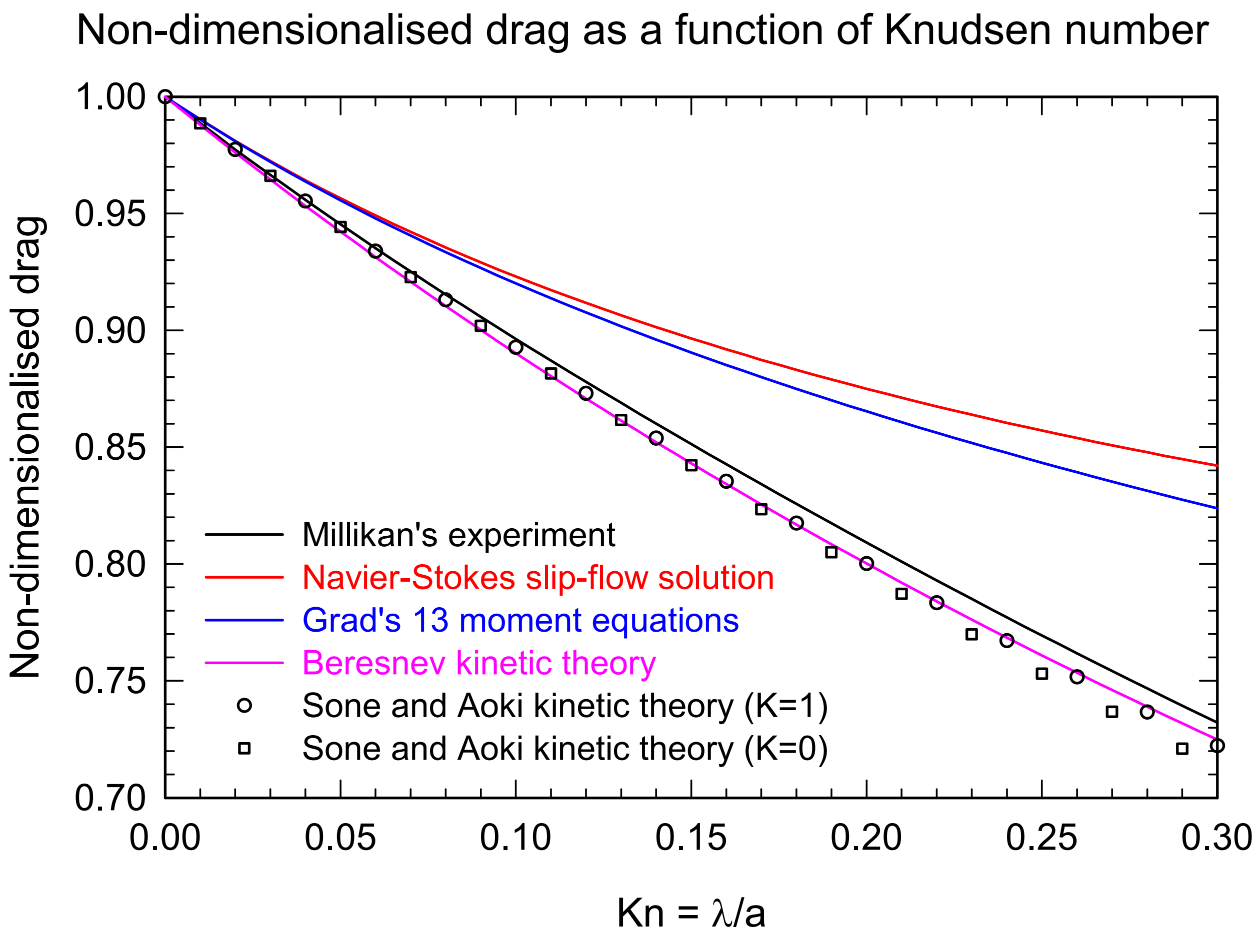


Failure to account for non-equilibrium effects (in particular, slip at the wall) results in the mass flow rate being underestimated by 40%.

Helium mass flow data:

E.B. Arkilic, M.A. Schmidt and K.S. Breuer, "Gaseous slip flow in long micro-channels", *J.M.E.M.S.*, 6(2) 167-178 (1997).

Comparison of non-dimensionalised drag force



a = radius of sphere

The challenge:
How can we extend the NSF equations?

Method of Moments (MoM)

Method originally developed by Harold Grad: Commun. Pure Appl. Math. (1949)

More macroscopic variables in addition to the conventional hydrodynamic variables

Original work stalled due to complexity of the 13-moment equations

Pioneering work by Struchtrup and Torrilhon created a regularized set of equations[1]

Work extended to include wall boundary conditions and computational strategy[2]

Work extended to 26-moments to capture correct physics of transition flow[3]

MoM can provide a bridge between kinetic theory and continuum mechanics in the transition regime

(1) Macroscopic Transport Equations for Rarefied Gas Flows, by *H. Struchtrup,* Springer (2005).

(2) X. J. Gu & D. R. Emerson, Journal of Computational Physics, V225 (1), pp. 263-283 (2007)

(3) X. J. Gu & D. R. Emerson, Journal of Fluid Mechanics, V636, pp. 177-216, (2009)

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Wall boundary conditions

Macroscopic wall boundary:

Velocity slip:

$$u_\tau = -\frac{2-\alpha}{\alpha}\sqrt{\frac{\pi RT}{2}}\frac{\sigma_{n\tau}}{p_\alpha} - \underline{\frac{5m_{nn\tau}+2q_\tau}{10p_\alpha} + \frac{9\Omega_\tau + 70\psi_{nn\tau}}{2520p_\alpha RT}}$$

Temperature jump

$$RT - RT_w = -\frac{2-\alpha}{\alpha}\sqrt{\frac{\pi RT}{2}}\frac{q_n}{2p_\alpha} - \underline{\frac{RT\sigma_{nn}}{4p_\alpha} + \frac{u_\tau^2}{4} - \frac{75R_{nn}+28\Delta}{840p_\alpha} + \frac{\phi_{nnnn}}{24p_\alpha}}$$

Tangential heat flux

$$q_\tau = -\frac{5}{18}\frac{2-\alpha}{\alpha}\sqrt{\frac{\pi RT}{2}}\left(7\sigma_{n\tau} + \frac{R_{n\tau}}{RT}\right) - \frac{5\hat{u}_\tau p_\alpha\sqrt{RT}\left(\hat{u}_\tau^2 + 6\hat{T}_w\right)}{18} - \frac{10m_{nn\tau}}{9} - \frac{5\psi_{nn\tau}}{81RT} - \frac{\Omega_\tau}{56RT}$$

Gu & Emerson, J. Fluid Mech. (2009)

....

A comment on computational cost

Research goal: develop computable approaches that are suitable for engineering applications and can reliably capture nonequilibrium effects

Microscopic approaches

Most popular approach is the direct simulation Monte Carlo (DSMC) method

Simulate the molecules movements and interactions directly using simulation molecules which represent a large number of real molecules.

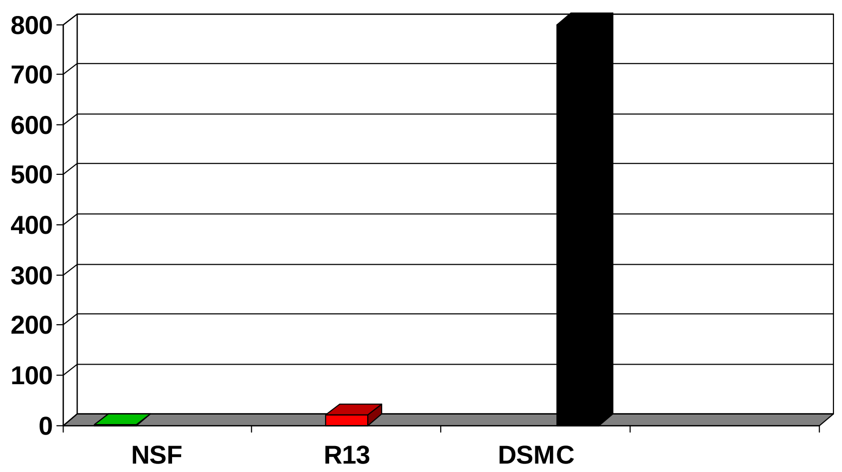
The fundamental assumption of the DSMC method is that the molecular movement and collision phases can be decoupled over time periods that are smaller than the mean collision time.

Powerful, complicated molecules, chemical reactions

Stochastic nature, statistical noise

Benchmarks for macroscopic models

Bird (1994) Molecular gas dynamics and the direct simulation of gas flows.



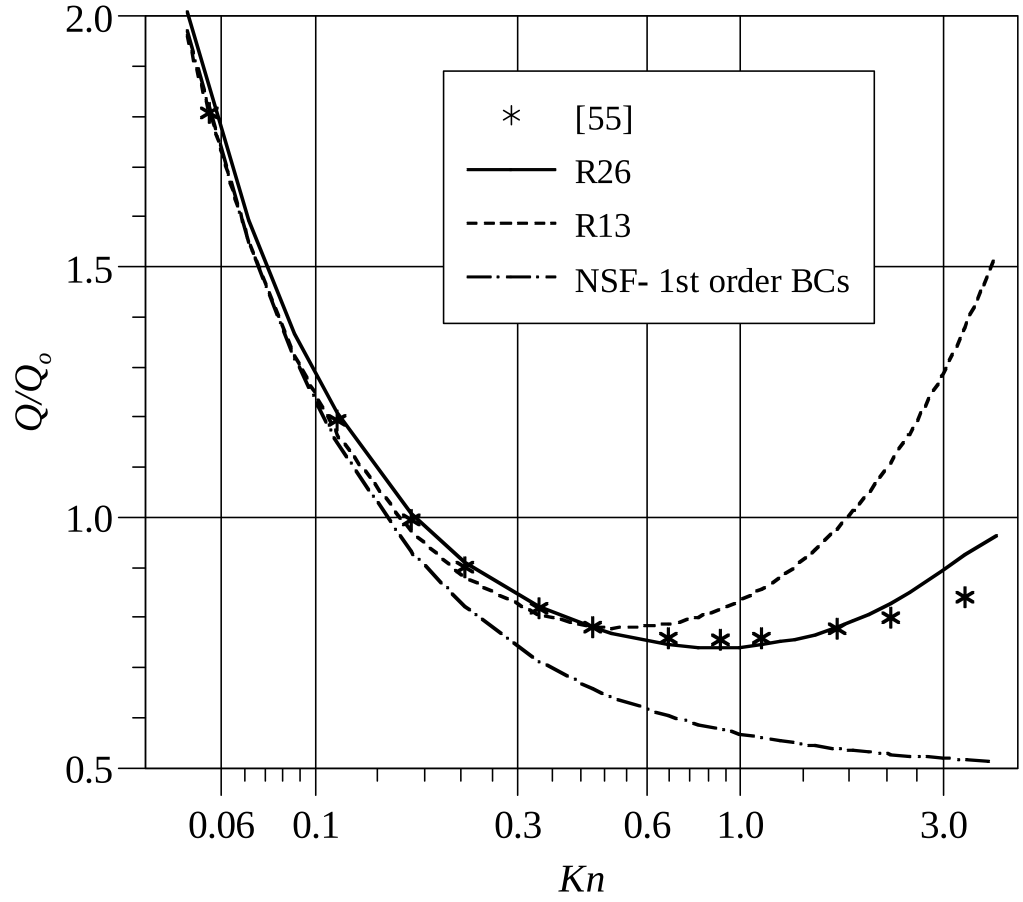
From an engineering point of view, it is important to validate the reduced macroscopic models against various non-equilibrium phenomena to examine their capabilities as well as limitations before the models are employed on real applications

- Knudsen minimum
- Kramers' problem
- Planar Couette flow
- Fourier flow
- Poiseuille flow: *pressure driven*
  force driven
- Cylindrical Couette flow
- Oscillatory flow
- Driven cavity flow
- Eccentric circular cylinder flow
- Knudsen pump
- Extended Graetz problem

Knudsen minimum

Figure shows how a range of codes perform trying to capture a well-known non-equilibrium phenomena known as the Knudsen minimum.

This is an important comparison against kinetic theory and the R26 equations perform very well.



Kramers' problem

A defect velocity is defined by $\boxed{u_d = \bar{y} + \zeta - \tilde{u}}$

The slip coefficient is determined by $\boxed{\lim_{\bar{y}\to\infty} u_d = 0}$

LR26 equations

$$u_d = -\frac{2-\alpha}{\alpha}\left(C_1 e^{-1.212\sqrt{\pi/2}\bar{y}} + 0.178 C_2 e^{-0.594\sqrt{\pi/2}\bar{y}}\right)$$

$$\zeta = \frac{2-\alpha}{\alpha}\left(1 - 0.5C_1 - 0.117C_2\right)$$

LR13 equations

$$u_d = \frac{2-\alpha}{\alpha}\left[\frac{\alpha e^{-\sqrt{5\pi/18}\bar{y}}}{\left(6-\sqrt{10\pi}\right)\alpha + 2\sqrt{10\pi}}\right]$$

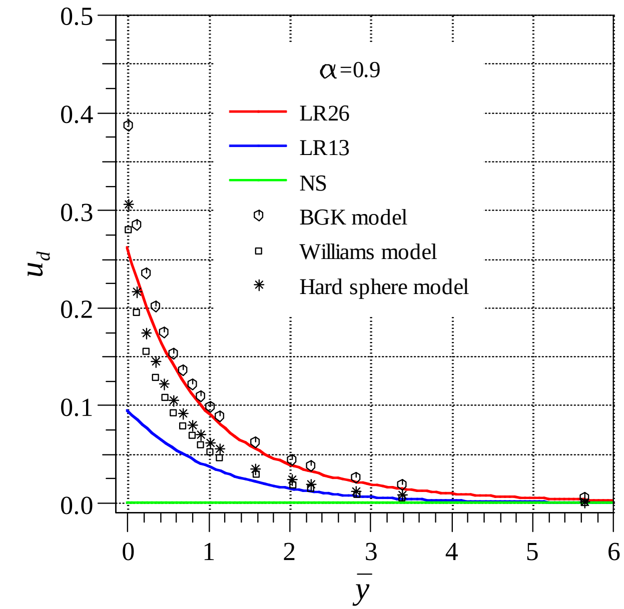
$$\zeta = \frac{2-\alpha}{\alpha}\left[\frac{\left(13-2\sqrt{10\pi}\right)\alpha + 4\sqrt{10\pi}}{\left(12-2\sqrt{10\pi}\right)\alpha + 4\sqrt{10\pi}}\right]$$

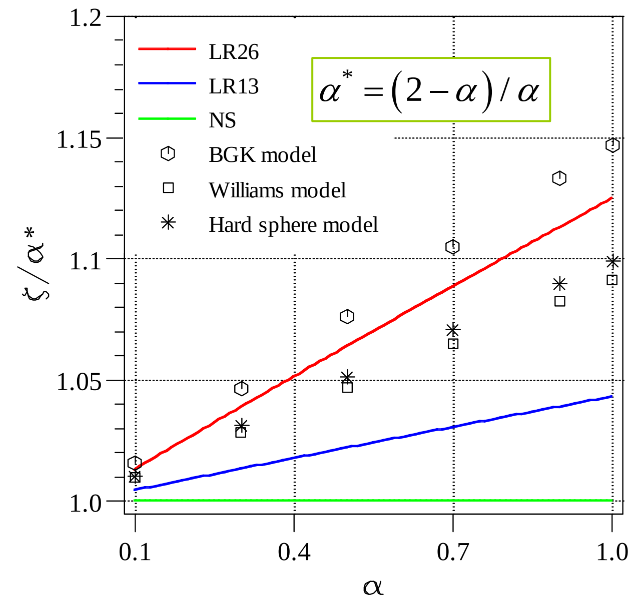
NS equations

$$u_d = 0,$$

$$\zeta = \frac{2-\alpha}{\alpha}.$$

Siewert (2001) *Euro. J. Appl. Math.* 12:179-191





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Compressible viscous flow simulation for arbitrary geometries using FLASH Code

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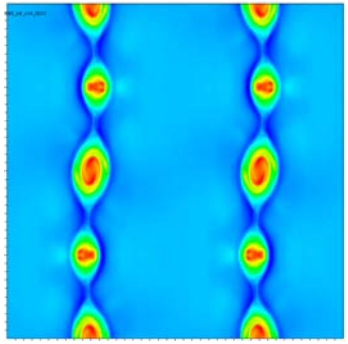
Joint Daresbury/Jülich Supercomputing Centre Meeting, Jülich, May 7-8 (2013)

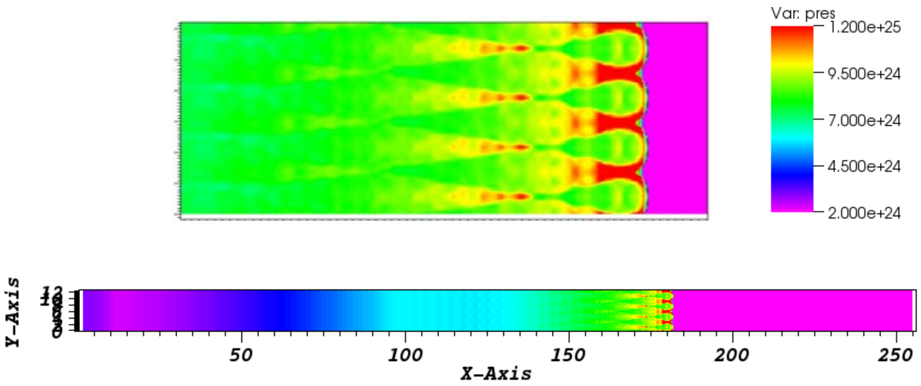
FLASH Code

- ❑ Parallel, adaptive-mesh refinement (AMR) code
  - – maintained by Flash Center, University of Chicago
- ❑ Designed for compressible reactive flows
- ❑ Can solve a broad range of problems
  - – hydrodynamics to MHD, nuclear & astrophysical problems

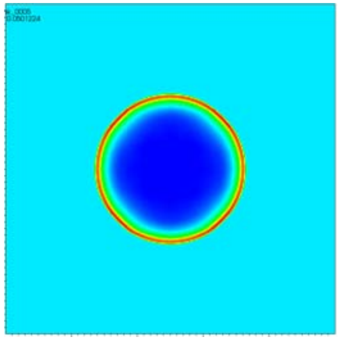


Current density field

Magnetohydrodynamics (MHD)



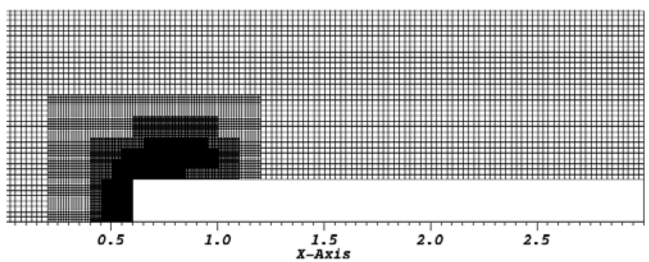
Detonation front (pressure field) in cellular nuclear burning

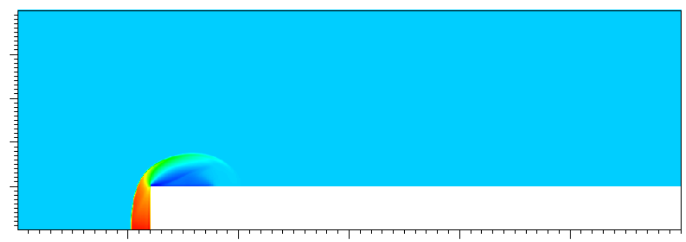


Sedov blast problem

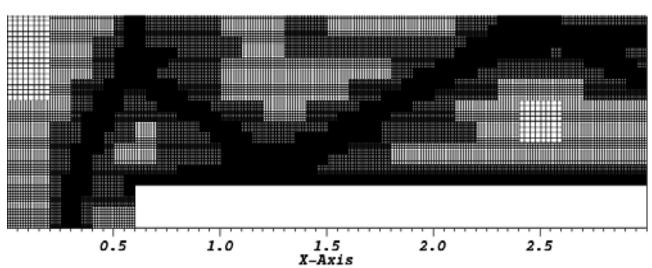
Adaptive Mesh Refinement (AMR) capability

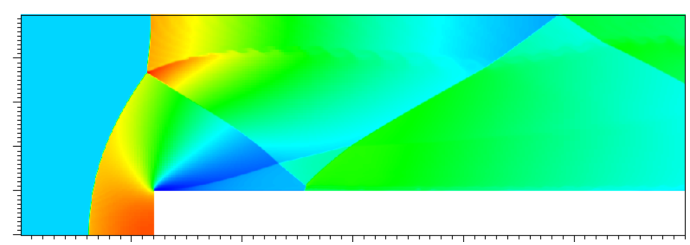
- Required due to the large range of length scales
- Resolution only where it is needed – can handle large problems
- PARAMESH & CHOMBO libraries in FLASH 4





t = 0.1 s





t = 4.0 s

Wind Tunnel-step problem using inviscid solver at Mach 3

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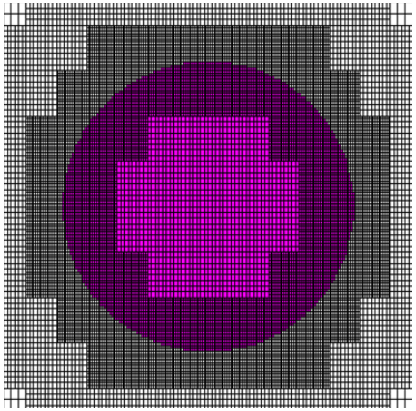
Extension of FLASH code for flow past arbitrary geometries

Current FLASH Capabilities

• Compressible FVM hydro solver : dimensionally split (PPM) & unsplit (MUSCL) solvers
 - various Riemann solvers, slope limiters, discretization schemes etc.

• Flow-past-rigid-body scheme in FLASH 4 limited to simple shapes
 - body surface represented by stair steps pattern

• Originally for astrophysics, where viscous-wall effects unimportant
 - hydro solutions limited to Euler equations


AMR mesh

Implemented in FLASH

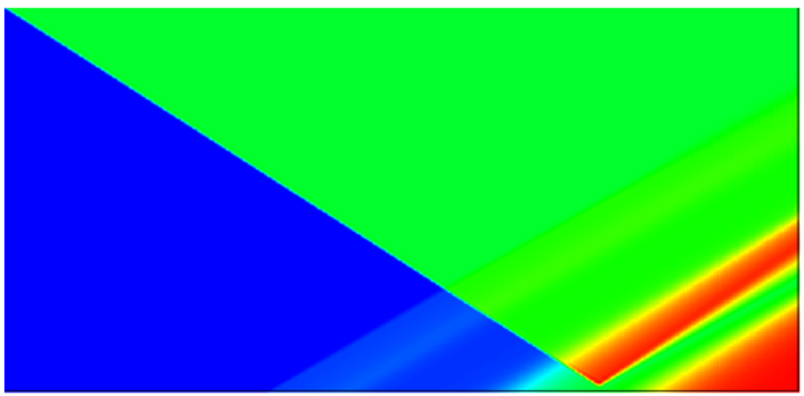
• Computer graphics algorithms to generate any random 3d or 2d shapes
 - based on a point-in-polyhedron test using spherical polygons by Carvalho & Cavalcanti

• Wall boundary conditions for viscous-wall interactions
 - no-slip boundary conditions & Sutherland viscosity law

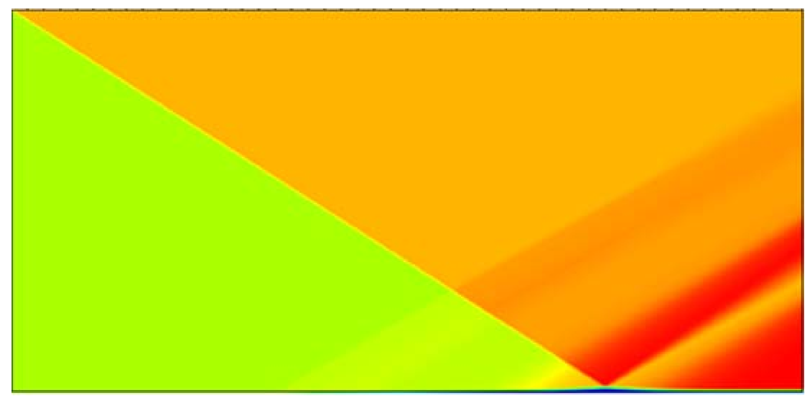
Validation of Navier-Stokes implementation in FLASH

(2D Shock boundary layer interaction (SBLI) case: Ma=2, Re = 2.96e5, Shock angle =32.6 degrees)

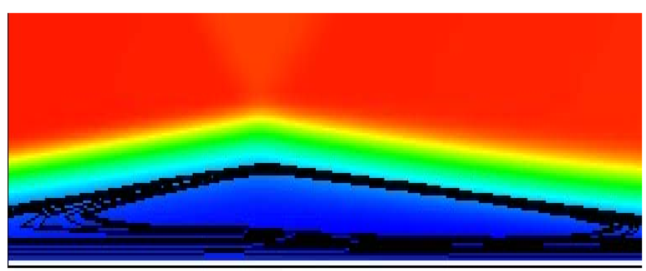
Pressure contours



Density contours



Streamlines near SBLI separation region



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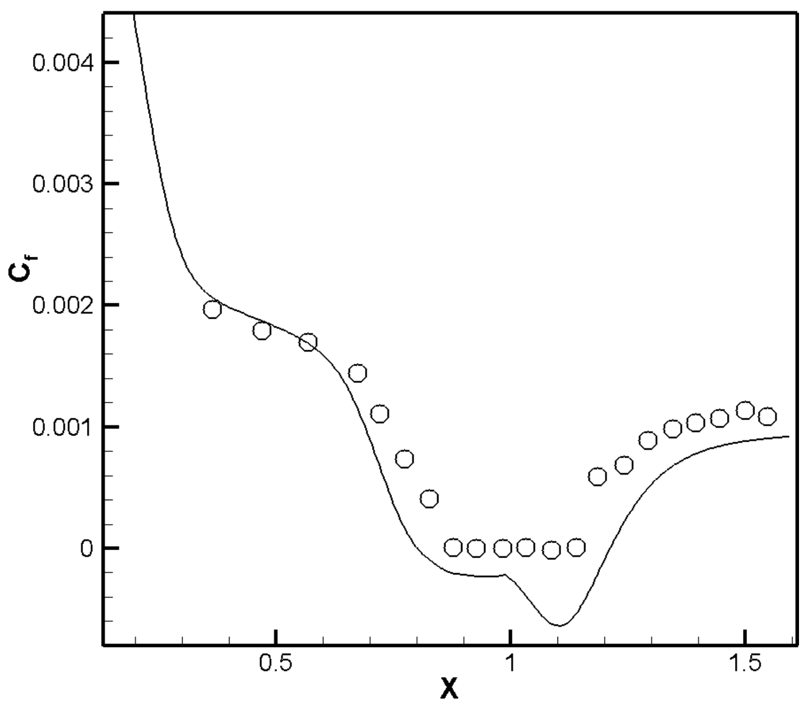
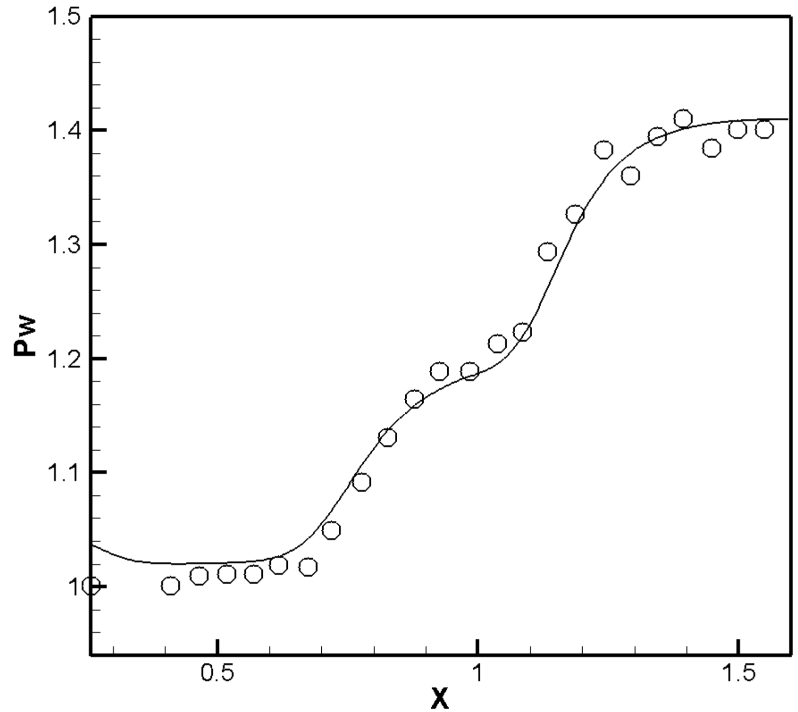
Validation of flow variables along the wall

(2D SBLI case: Ma=2, Re = 2.96e5, Shock angle =32.6 degrees)

Skin friction coefficient



Wall pressure

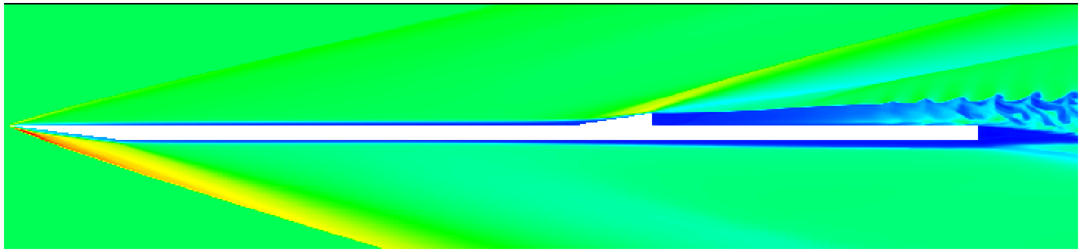


Comparison with experimental data from Hakkinen et al.

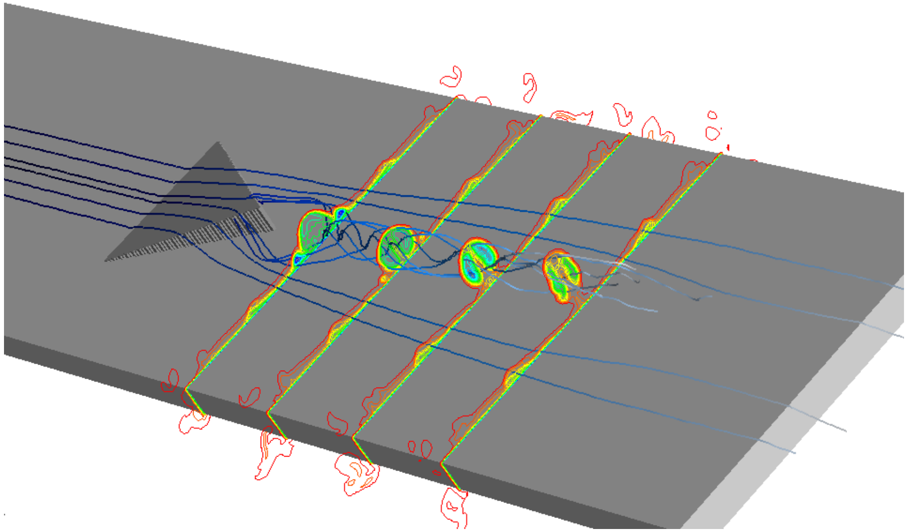
Hypersonic flow control using Micro Vortex Generator

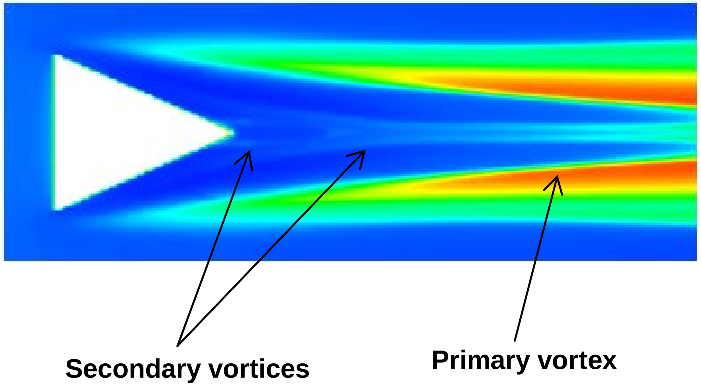
(Navier-Stokes solution at Mach 5 **without** shock generator)

Density field



Density contours





Collaboration with U. Manchester (Kontis)

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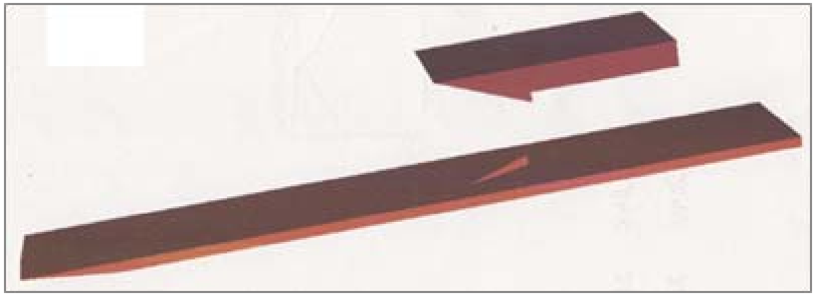
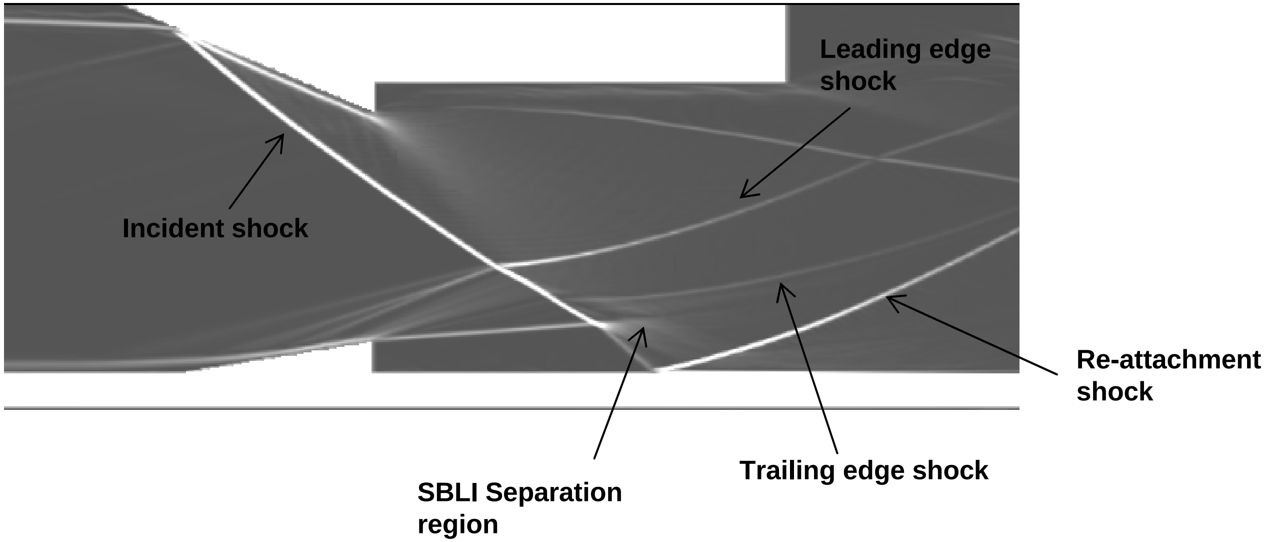
Hypersonic MVG Simulation with Shock generator

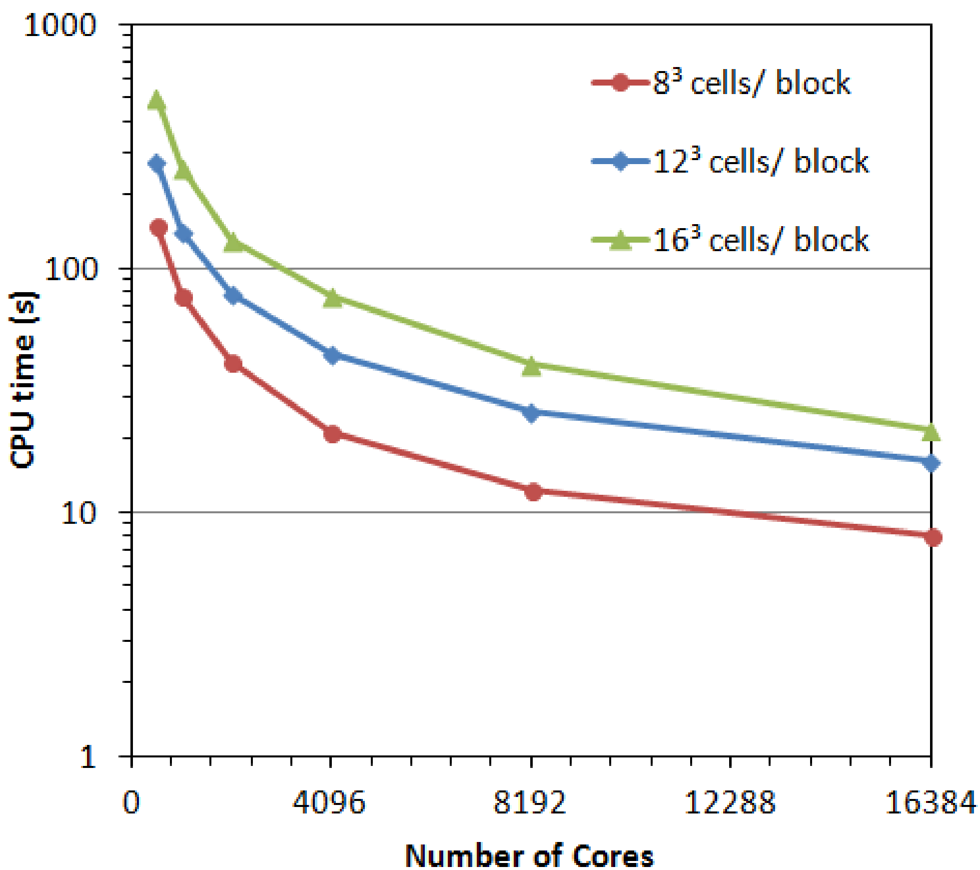
Model setup for MVG with shock generator



Numerical Schlieren showing shock-boundary layer interaction



FLASH Scalability on Blue Gene/Q for MVG simulation



Summary & Future work

- Computer graphics algorithms implemented in FLASH code to enable flow simulation past any arbitrary 3D geometric shape
- Viscous-wall boundary conditions implemented for Navier-Stokes solutions
- NS implementation validated for a 2D SBLI case
- 3D Hypersonic MVG simulations carried out – all basic flow features captured
- More validations to be done and additional capabilities will be made in FLASH

Environmental fluid dynamics

High Resolution Hydrodynamic Study of the River Rhine: from the City of Bonn to the North Sea

Thanks to R. KOPMANN

Bundesanstalt für Wasserbau, Karlsruhe, DE

Motivation

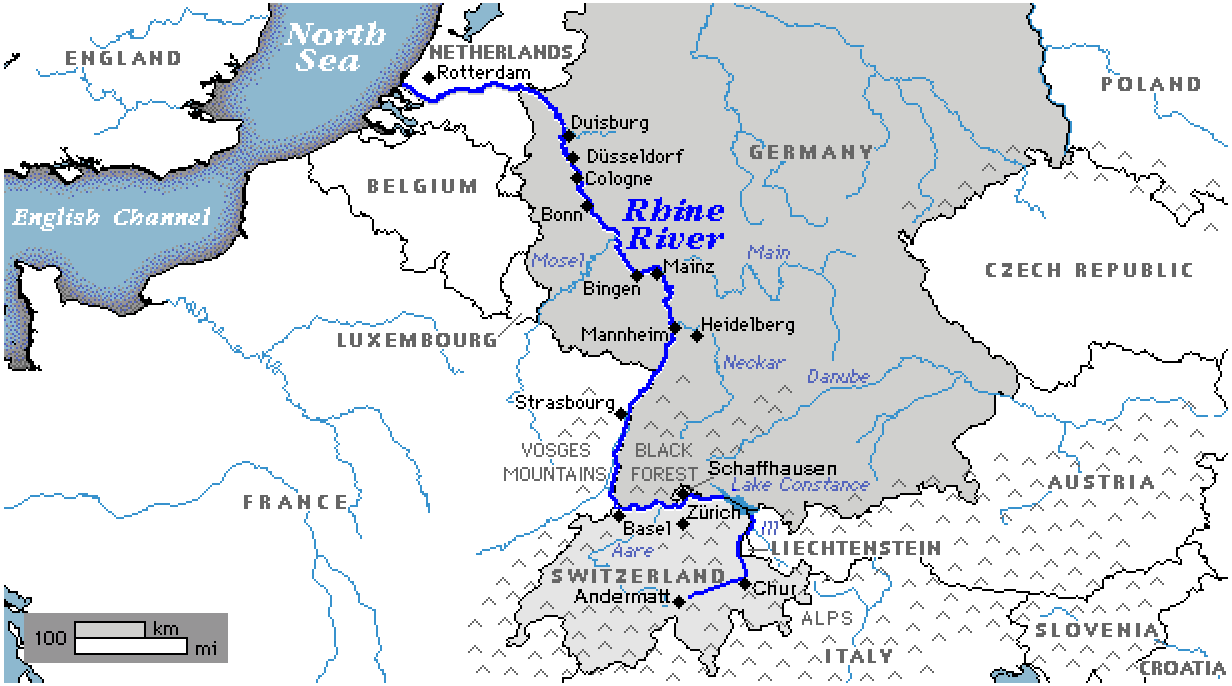
2D hydrodynamic simulations (finite elements method) usually utilise coarse grids for several reasons:-
- accurate bathymetry might not be available,
- long-term scenarios of sometimes several months/years need to be performed.

We are exploring how Telemac can deal with a very large simulation of over 4M elements (current typical grid size of the order of a hundred thousand elements).

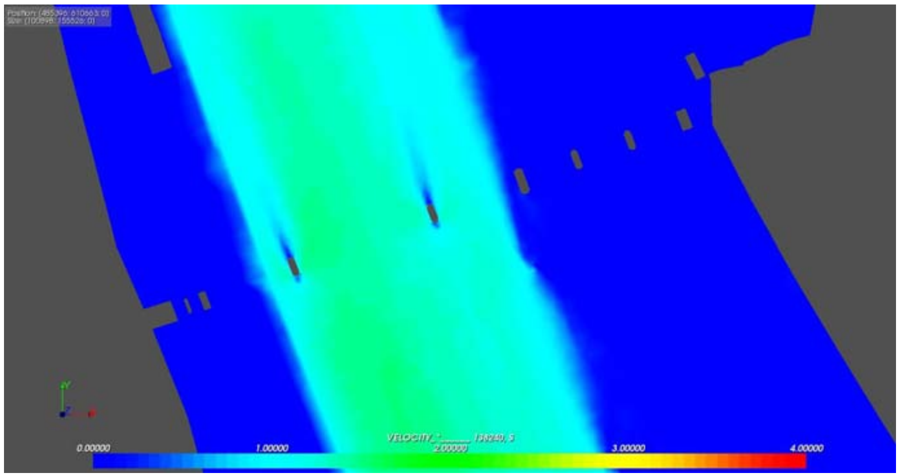
A feasibility study of the Rhine River is currently underway.
Accurate bathymetry is available at BAW, coming from several sources:
1 - photogrammetric measurements,
2 - soundings from 2006 cross sections,
3 - the German map of the federal waterways,
4 - geo-referenced aerial pictures, and
5 - Laserscan-data sets with 2* 2m raster from 1998 for the flood plane area (Rhine-km 657.1 to Rhine-km 660.0).

Motivation

The hydrodynamics of the five contiguous parts were calibrated individually at a levelling from September 2001 and the same calibration was used for the assembled model. Thereby 10 different roughness zones (for the river channel, groynes, banks, floodplains, farmland, grassland, special zones, forests, harbours and other water bodies) were distinguished during the calibration.

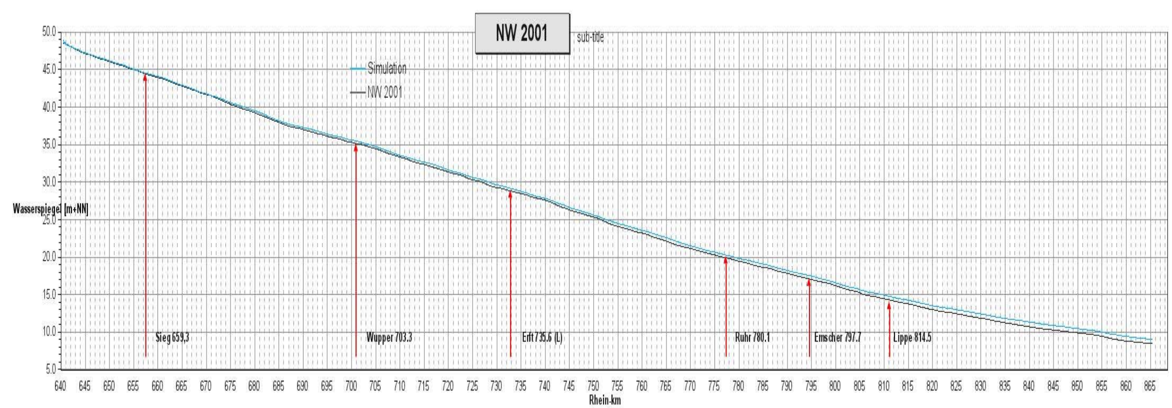


Very preliminary results



Snapshot of the flow under a bridge capturing flow separation

Simulated water levels compared to the measured ones from September 2001



Comments

- Other key projects (not mentioned)
  - Network in Meshfree Methods (with Ben Rogers & Stephane Bordas)
  - Programme Grant investigating multiscale coupling with MD/CFD
  - Strategies for petascale & exascale CFD
  - Future-proof multiblock capability
  - Biomimetic micro-channel designs…….

An Overview of Computational Engineering at Daresbury

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