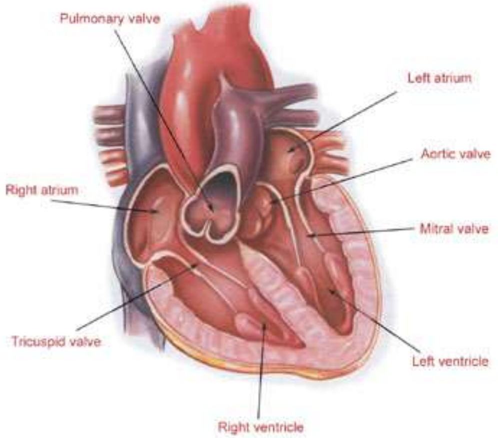
Tutorial School on Fluid Dynamics: Topics in Turbulence May 24-28, 2010



Methodologies & Applications

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Outline

- Introduction
- Methodologies
  - Problem Formulation
  - Fluid-structure interactions in LES
  - Embedded Boundary Method
- Applications
  - Internal Flows (cardiovascular circulation)
    - Flow in stenotic arteries
    - Flow around prosthetic heart valves
- Summary and Future Research

Introduction

What are biological flows?

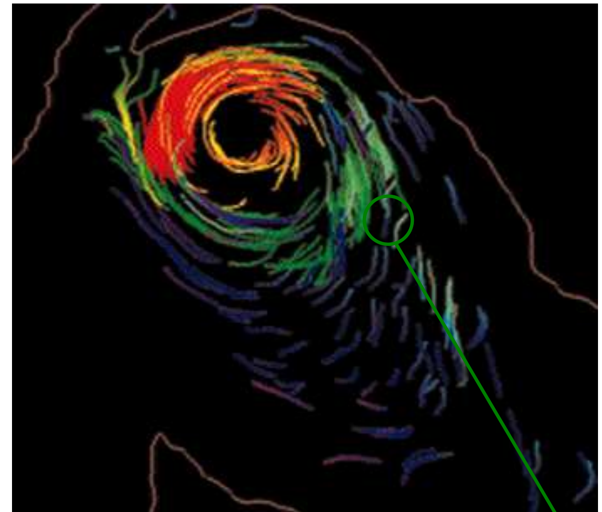
Example 1: The human body, where fluids *play a critical role, i.e.*

- Respiratory system
- Circulatory system
- ……….

A variety of flow phenomena at multiple scales:

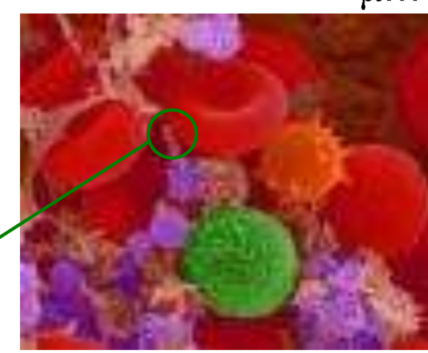
- Organ level (Re<8000)
- Cellular level
- Molecular level

cm



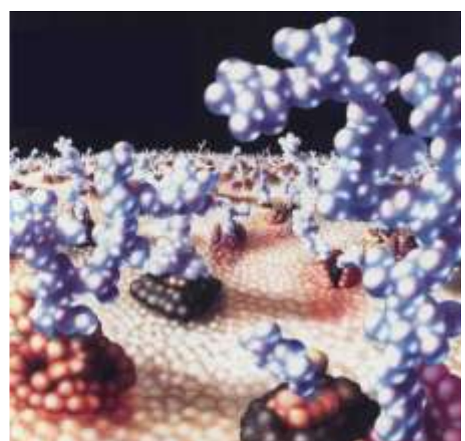
Flow patterns in the human aorta

μm



Blood elements

nm



Molecules on the cell surface

Introduction

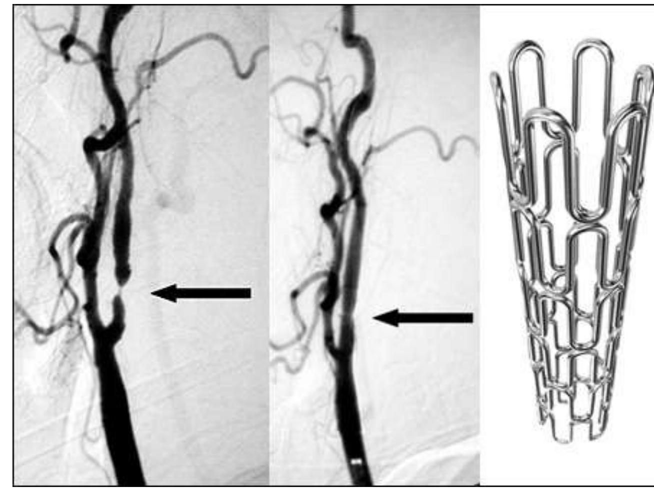
Is turbulence important in biological flows?

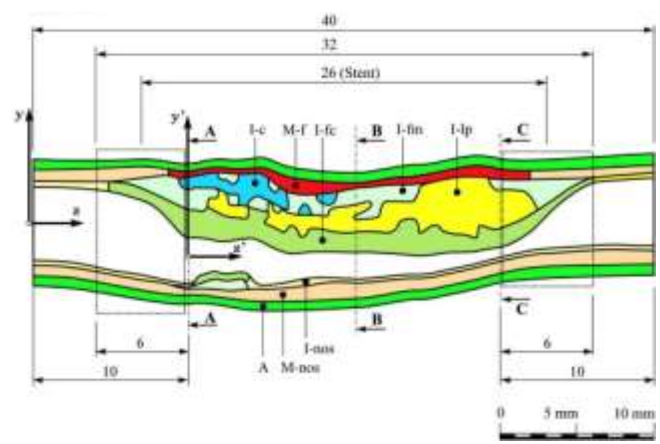
Example 1: Turbulence is the exception in the circulation. It appears in pathologic situations:

- Atherosclerosis
- Medical implants can trigger turbulence
- Medical devices

Turbulence is not desirable in blood circulation: DNS/LES can help understand and control (avoid) it

- Disease research
- Surgical Planning
- Devise Design





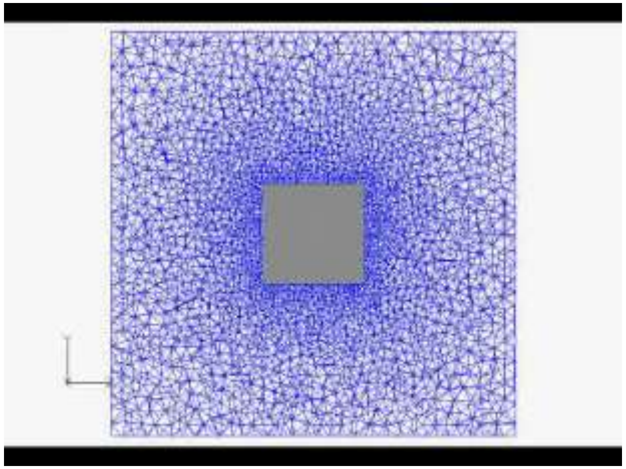
Introduction

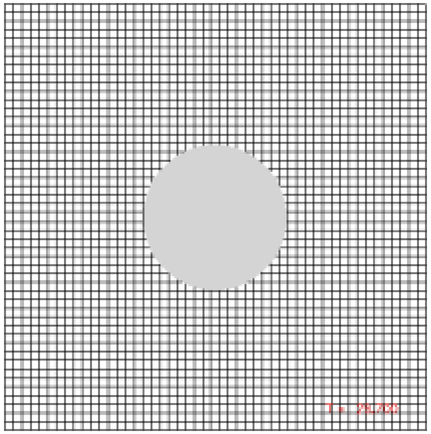
Core of modeling tools: FSI NS-solver for incompressible flow

Critical elements:

- Treatment of moving boundaries
  - AMR solver
  - Non-boundary conforming
- Modeling turbulence/transition
  - DNS/LES
  - Fidelity and conservation properties
- Coupling/modularity
  - Different structural solvers (i.e non-linear 3D beam, plate/shell etc.

Treatment of moving boundaries





Boundary conforming

- Grid deformation is required to satisfy the conformation constrain
- Equations need to be modified to account for relative motion to the grid
- Flexible in clustering grid points
- For large deformations grid quality is an issue for stability and efficiency

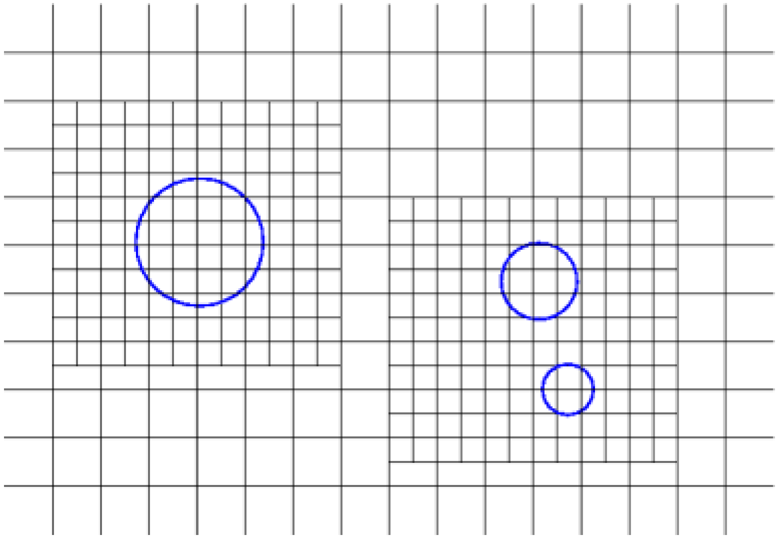
Non-Boundary conforming

- A fixed Eulerian grid is used at all times
- Equations of motion remain unchanged
- Boundary conditions not trivial
- Quality of the solution does not depend on how large deformations are
- Inflexible in clustering grid points

Treatment of moving boundaries

Non-boundary conforming methods: variety of different schemes

- immersed boundary
- cut-cell
- direct forcing
- …….



Direct forcing based on moving-least-squares (MLS)*

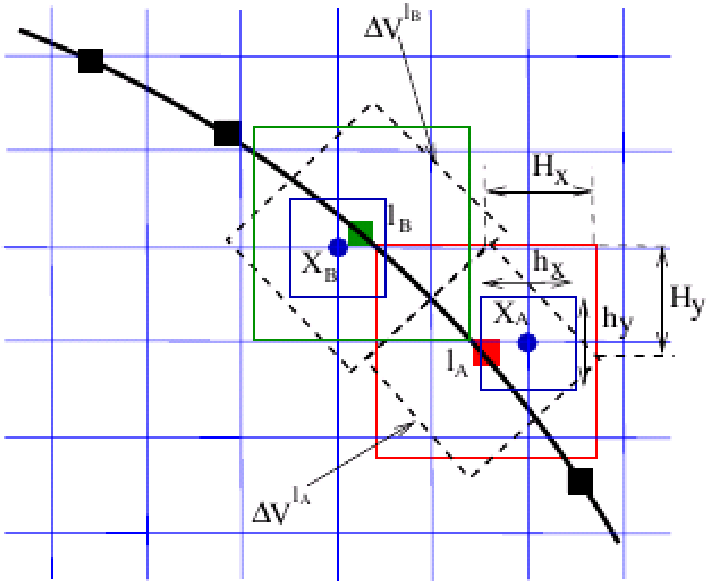
- Forcing is computed on Lagrangian markers
- MLS used to build transfer functions
- Does not depend on spatial discretization
- Does not compromise accuracy of the splitting scheme

**Vanella & Balaras, J. Comput. Physics, 2009*

MLS forcing scheme

Forcing can be computed on the Lagrangian markers:

$$F_i^{n+1/2} = \frac{U_i^d - U_i^n}{\Delta t} - RHS^{n+1/2}$$



Define the ‘predicted’ velocity on the markers:

$$\widetilde{U} = U_i^n + \Delta t\ RHS^{n+1/2}$$

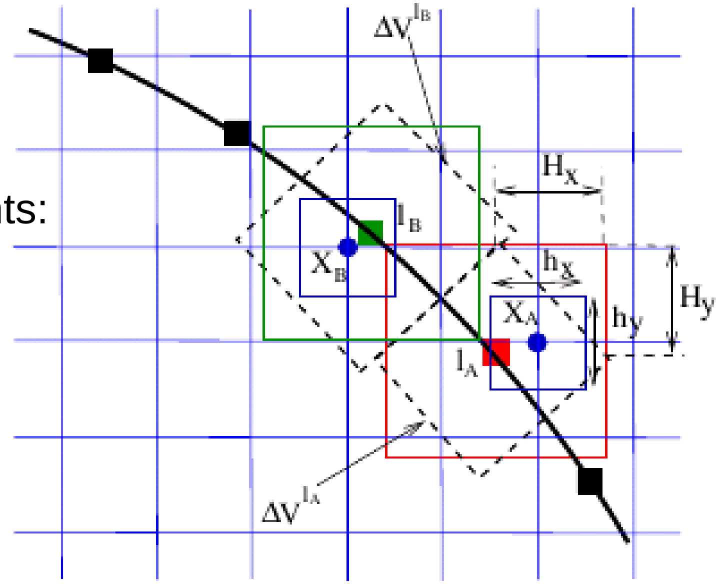
Then the forcing function on the the Lagrangian markers is:

$$F_i^{n+1/2} = \frac{U_i^d - \widetilde{U}_i}{\Delta t}$$

MLS forcing scheme

Build transfer functions for Largrangian/Eulerian grids

- Identify the closest Eulerian point to each marker
- Define support domain around each marker
- Associate a volume ΔV to each marker



We can approximate any variable on the Lagrangian points:

$$\widetilde{U}_i(\mathbf{x}) = \sum_{j=1}^{m} p_j(\mathbf{x}) a_j(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{a}(\mathbf{x})$$

where $\mathbf{p}^T(\mathbf{x})$ is the basis functions vector of length m,
$\mathbf{a}(\mathbf{x})$ is a vector of coefficients

To find the coefficients we can define the following weighted L_2 norm:

$$J = \sum_{k=1}^{ne} W\left(\mathbf{x} - \mathbf{x}^k\right)\left[\mathbf{p}^T(\mathbf{x}^k)\mathbf{a}(\mathbf{x}) - \tilde{u}_i^k\right]^2$$

$\mathbf{x}^k$ is the position vector of the Eulerian point k,
$\tilde{u}_i^k$ is the corresponding variable for grid point k
$W\left(\mathbf{x} - \mathbf{x}^k\right)$ is a given weight function

MLS forcing scheme

We minimize J with respect to **a(x)**:

$$\begin{aligned}
\mathbf{A}(\mathbf{x})\,\mathbf{a}(\mathbf{x}) &= \mathbf{B}(\mathbf{x})\,\tilde{\mathbf{u}}_i^k \quad \text{with,}\\
\mathbf{A}(\mathbf{x}) &= \sum_{k=1}^{ne} W(\mathbf{x}-\mathbf{x}^k)\mathbf{p}(\mathbf{x}^k)\mathbf{p}^T(\mathbf{x}^k),\\
\mathbf{B}(\mathbf{x}) &= [W(\mathbf{x}-\mathbf{x}^1)\mathbf{p}(\mathbf{x}^1) \;\cdots\; W(\mathbf{x}-\mathbf{x}^{ne})\mathbf{p}(\mathbf{x}^{ne})], \quad \text{and}\\
\tilde{\mathbf{u}}_i^k &= [\tilde{u}_i^1 \;\cdots\; \tilde{u}_i^{ne}]^T.
\end{aligned}$$

For linear basis functions **A(x)** is a 4x4 matrix. Cubic splines are used for the weight functions:

$$W(\mathbf{x}-\mathbf{x}^k) = \begin{cases} 2/3 - 4\overline{r_k}^2 + 4\overline{r_k}^3 & \text{for} \quad \overline{r_k} \le 0.5 \\ 4/3 - 4\overline{r_k} + 4\overline{r_k}^2 - 4/3\overline{r_k}^3 & \text{for} \quad 0.5 \le \overline{r_k} \le 1.0 \\ 0 & \text{for} \quad \overline{r_k} > 1.0 \end{cases}$$

MLS forcing scheme

We can now find the predicted velocity on the Lagrangian markers:

$$\widetilde{U}_i(\mathbf{x}) = \sum_{k=1}^{ne} \phi_k^l(\mathbf{x}) \tilde{u}_i^k = \mathbf{\Phi}^T(\mathbf{x}) \tilde{\mathbf{u}}_i^k$$

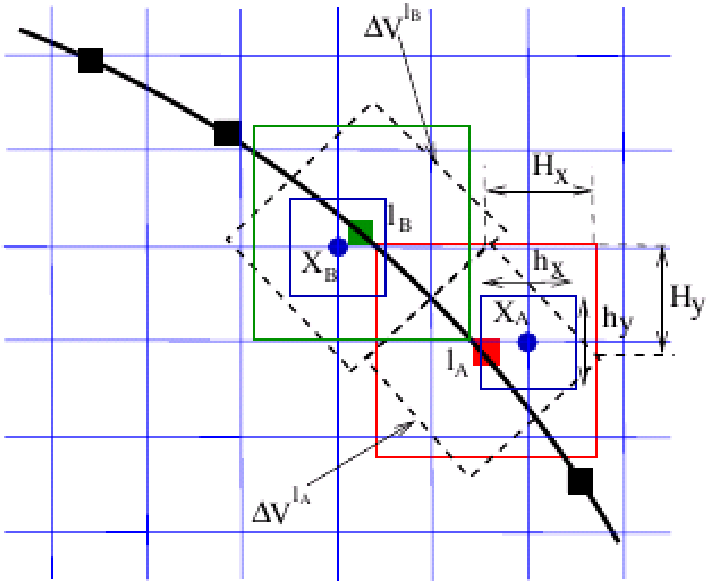
$\mathbf{\Phi}(\mathbf{x}) = \mathbf{p}(\mathbf{x})\ \mathbf{A}(\mathbf{x})^{-1}\ \mathbf{B}(\mathbf{x})$ is a column vector with length ne, containing the shape function values for marker point l.

The forcing on the Eulerian points would be:

$$f_i^k = \sum_{l=1}^{nl} c_l \phi_k^l F_i^l$$

nl is the number of markers associated to the Eulerian point. To compute c_l we require that the total force is not changed by the transfer:

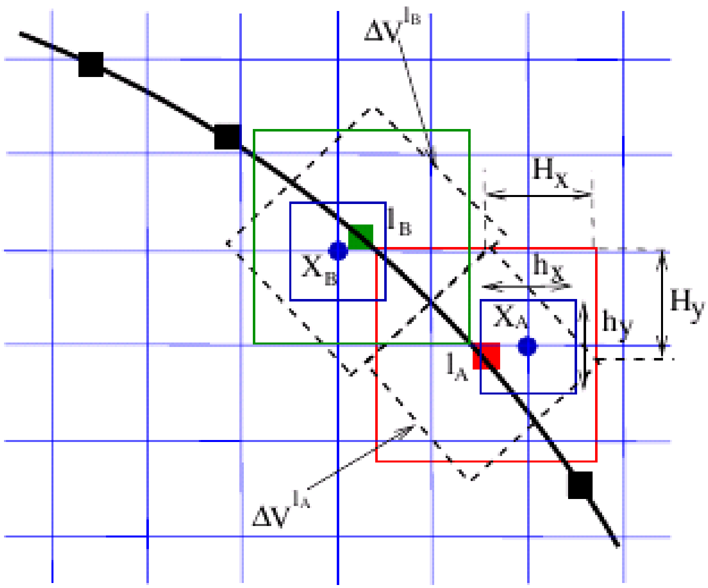
$$\sum_{k=1}^{nte} f_i^k \Delta V^k = \sum_{l=1}^{ntl} F_i^l \Delta V^l$$



MLS forcing scheme

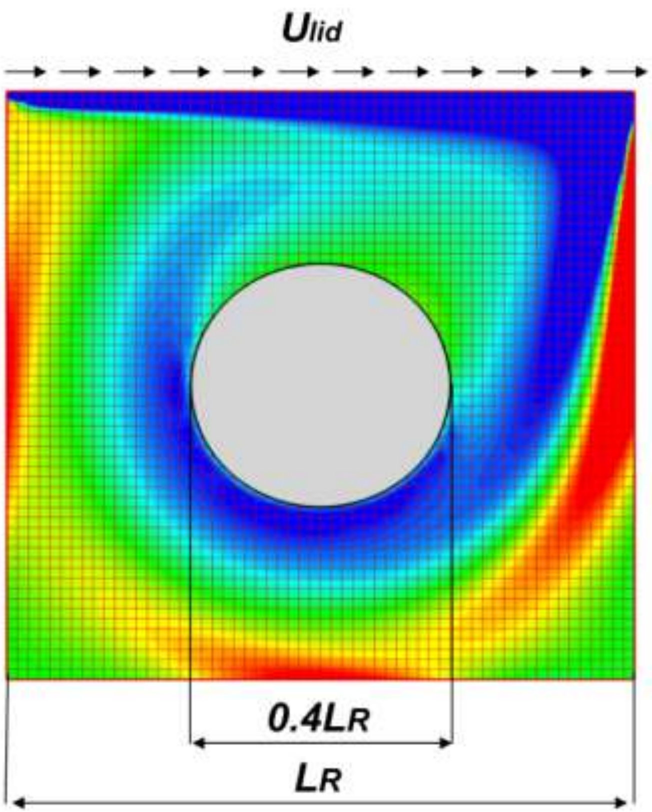
Basic characteristics of the MLS scheme:

- Conserves momentum and torque
- Very robust in treating multi-body moving boundary problems
- Transfer function build to arbitrary order of accuracy
- Can be combined with any numerical method
  - structured/unstructured
  - FD/FV/FE

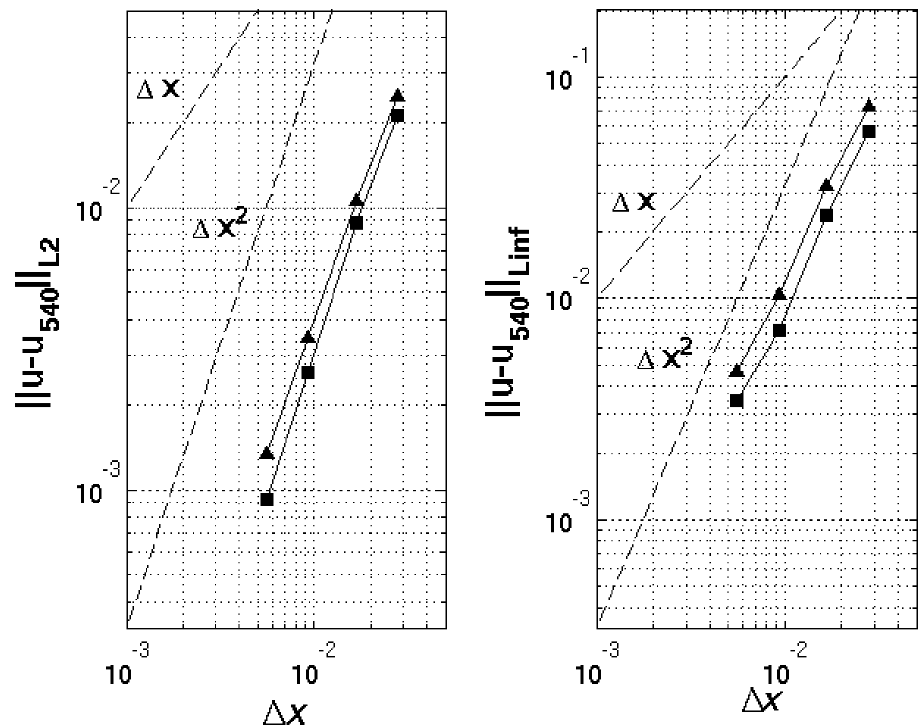


MLS forcing scheme

Accuracy study:



Cylinder in a cavity, Re=1000

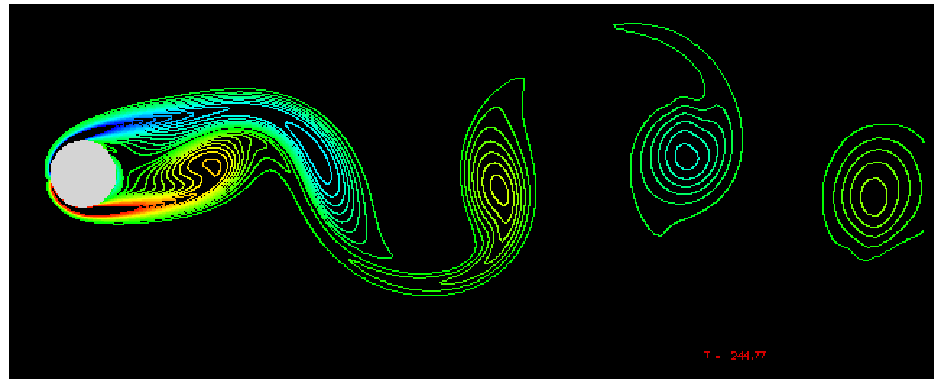


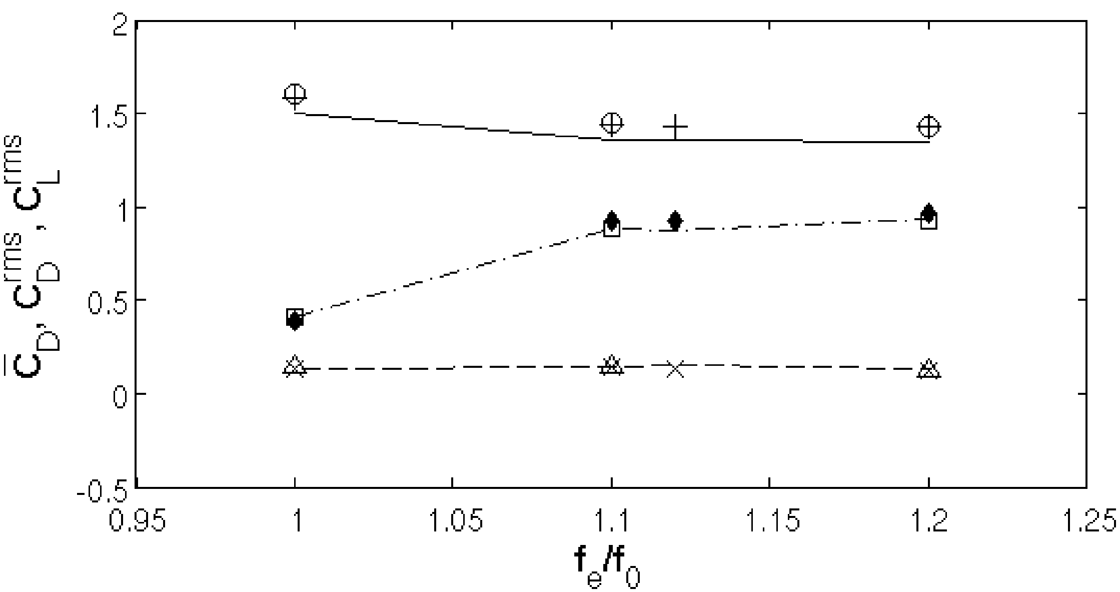
Error norms

MLS forcing scheme

Oscillating cylinder:

- Reynolds number:
  $\mathrm{Re} = UD/\nu = 185$
- Motion of cylinder:
  $y(t) = A\sin(2\pi f_e t)$

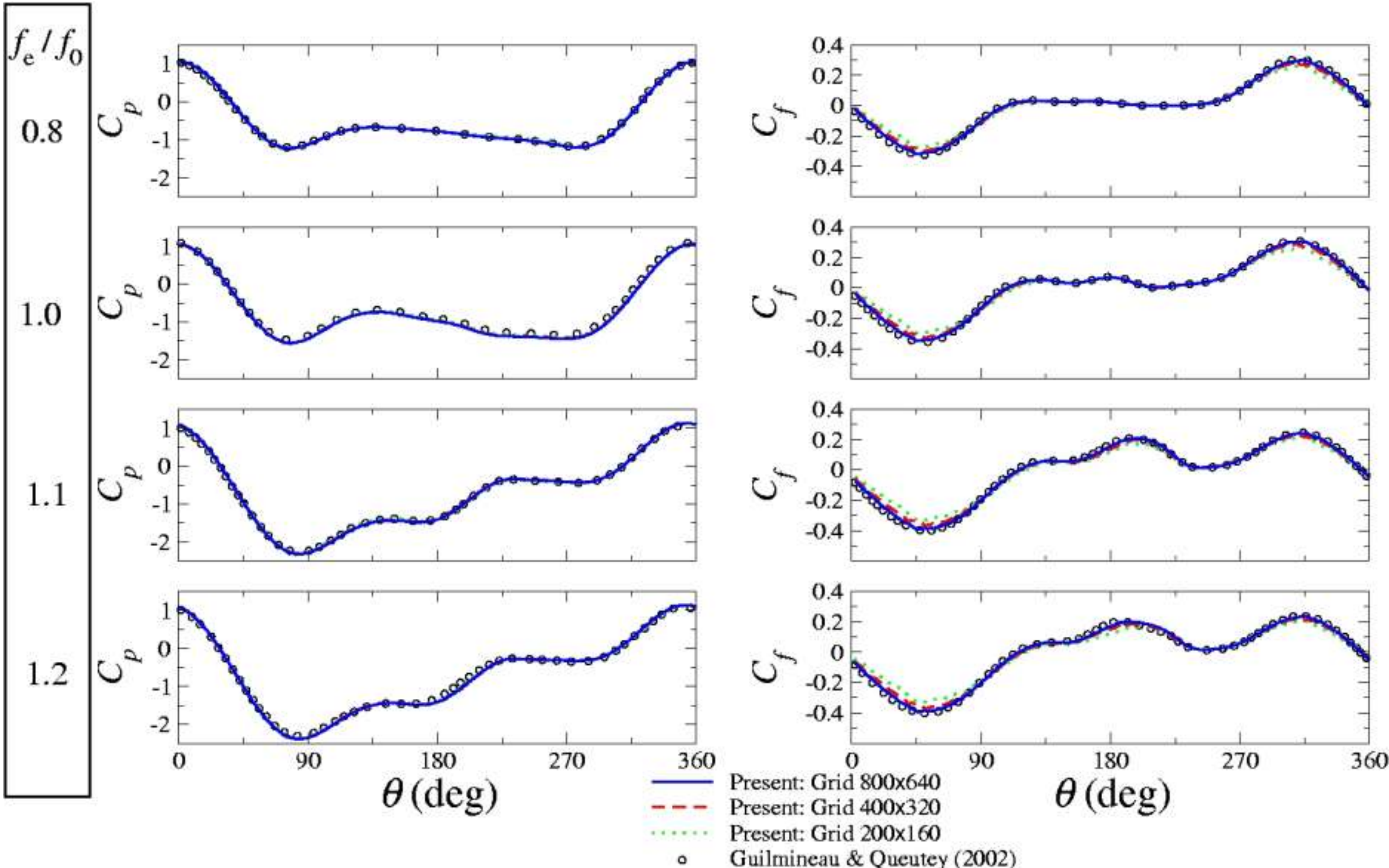




- Domain:
  $x: -10D \sim 40D$
  $y: -15D \sim 15D$
- Grids:
  200×160
  400×320
  800×640

MLS forcing scheme

Oscillating cylinder: force distribution on the surface



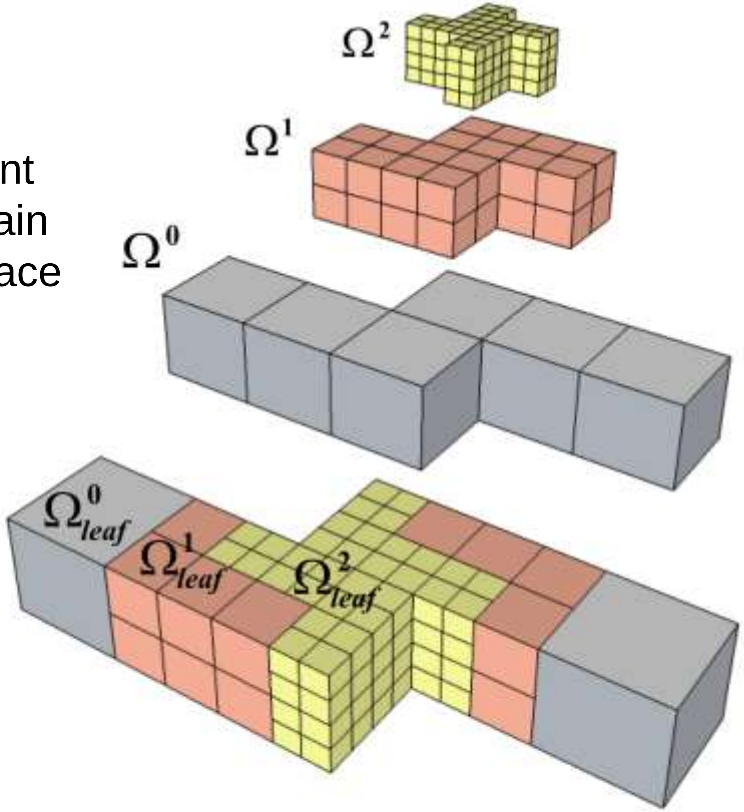
Parallel AMR NS-solver

- Immersed boundary approaches are usually tied to structured Cartesian grids that do not allow flexibility in grid refinement. As a results limited applicability to:
    - Problems with highly irregular boundaries undergoing large displacements/deformations
    - Moderate, large Reynolds numbers
- It is desirable to combine advantages of Cartesian grids with adaptively increasing resolution in particular zones of the flow domain.

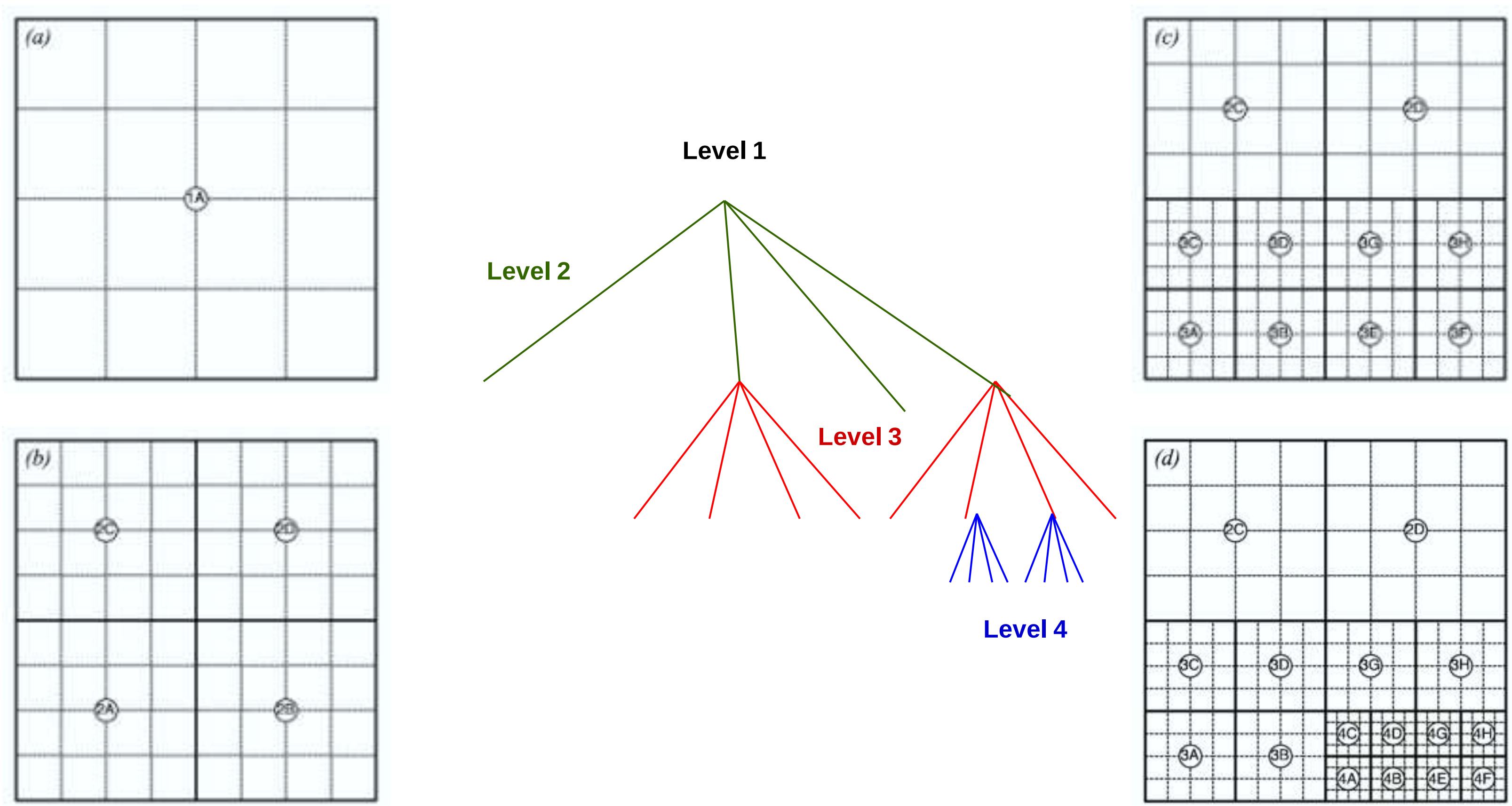
Parallel AMR NS-solver

An octree of blocks:

- Block structured
- All blocks have same dimensions
- Blocks at different level of refinement have different grid spacing and cover different portions of the domain
- Global block numbers based on Morton order (space filling behavior)
- Blocks have leaf-parent relation

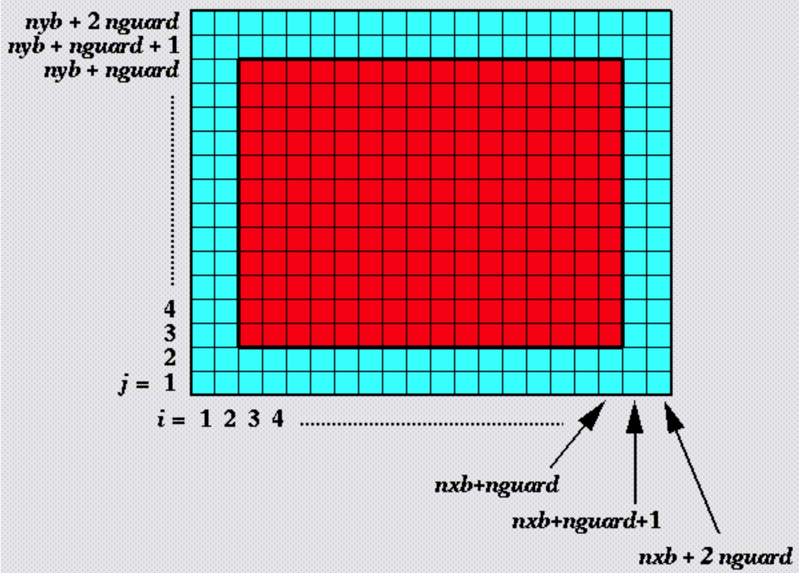


Parallel AMR NS-solver



Parallel AMR NS-solver

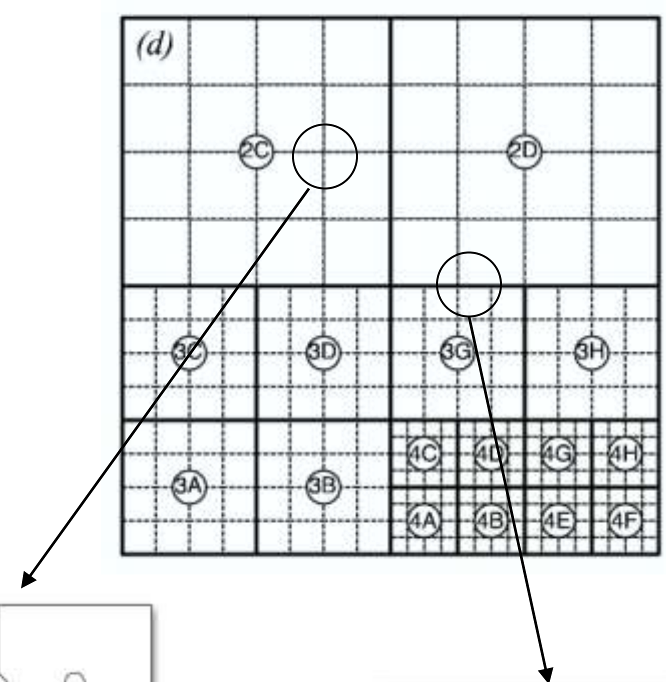
- grid composed of blocks
- all blocks have same size
- each block reserves space for layers of guard c

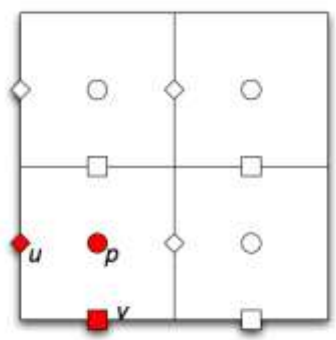


Indexing scheme for a 2D grid block with 2 guard cells (nguard=2) at each block boundary. Interior cells are colored red, guard cells are colored blue.

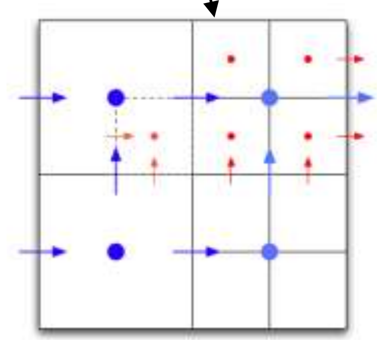
Parallel AMR NS-solver

- We use a **projection method**, where advective and diffusive terms are advanced explicitly
- We use the **Paramesh toolkit** (developed by MacNeice and Olson) for the implementation of the AMR process. The package creates and maintains the hierarchy of sub-grid blocks, with each block containing a fixed number of grid points.
- A **single-block Cartesian** grid solver is employed in each sub-grid block:
  - standard staggered grid in each sub-block
  - second-order central finite-differences
- A hybrid **direct/multigrid** solver is used for the **Poisson** equation (developed in collaboration with the **FLASH-Group**)
- **Guard cells** are used to discretize equations at the interior coarse-fine interfaces





standard staggered grid



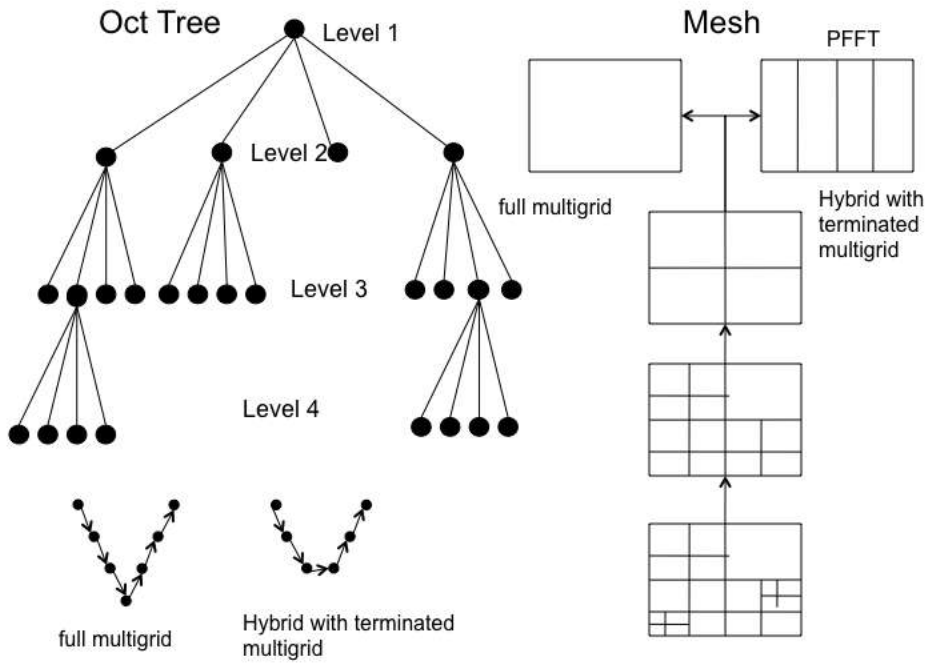
coarse-fine interface

Parallel AMR NS-solver

The multigrid algorithms have an inherent scaling limitation:

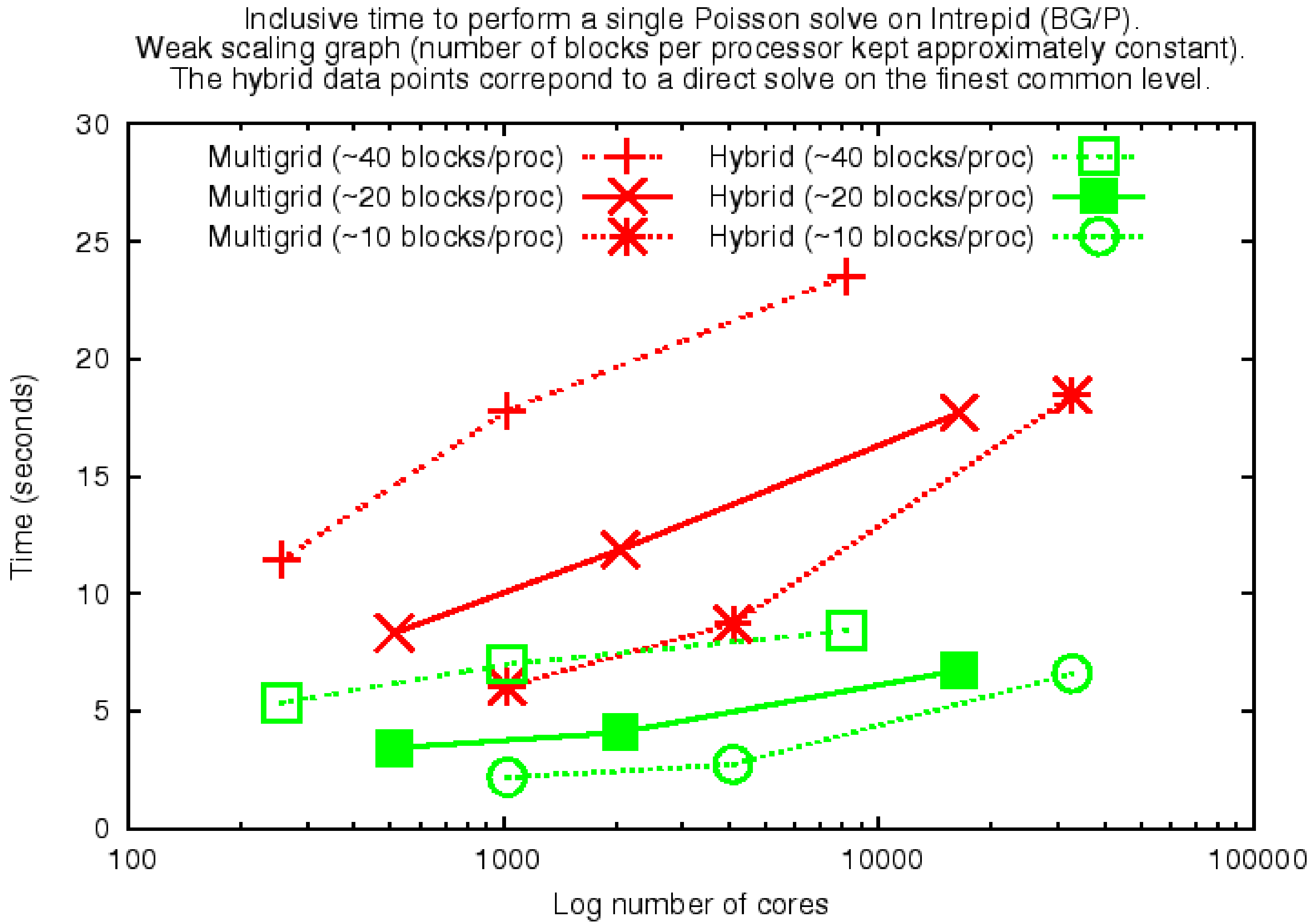
- as the grid gets coarser, there is less computational load to distribute among processors.
- as the number of blocks at a level approaches the number of processors, we begin to see the overhead cost of low computation/communication ratio.
- further reduction in the number of blocks, processors start to become idle and load balance deteriorates (at the coarsest level, very few processors are busy).

Parallel AMR NS-solver



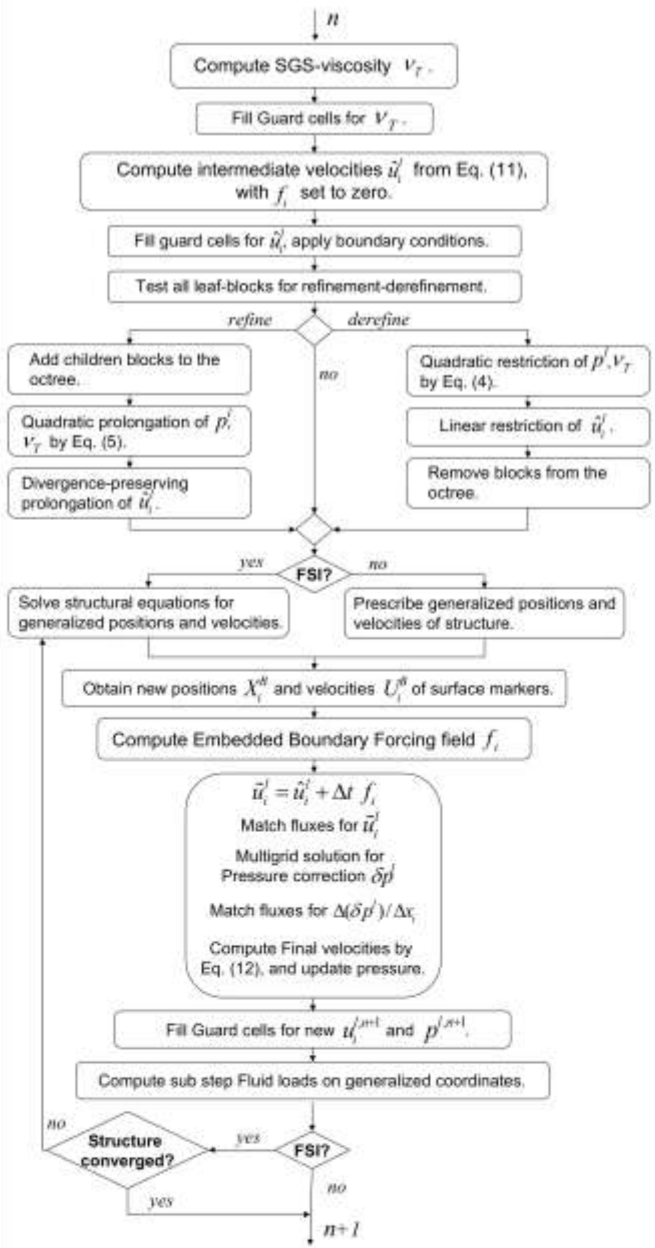
• we do not complete a V cycle, and instead coarsening of the grid is stopped at a predetermined level.
• the coarse level may be any level that is fully refined (i.e. containing blocks that completely cover the computational domain).
• The solution at this level is computed using one of the parallel direct solvers

Parallel AMR NS-solver



Vanella et al, J. Comput. Science, 2010

Parallel AMR solver: summary of algorithm



Adaptive mesh refinement: accuracy

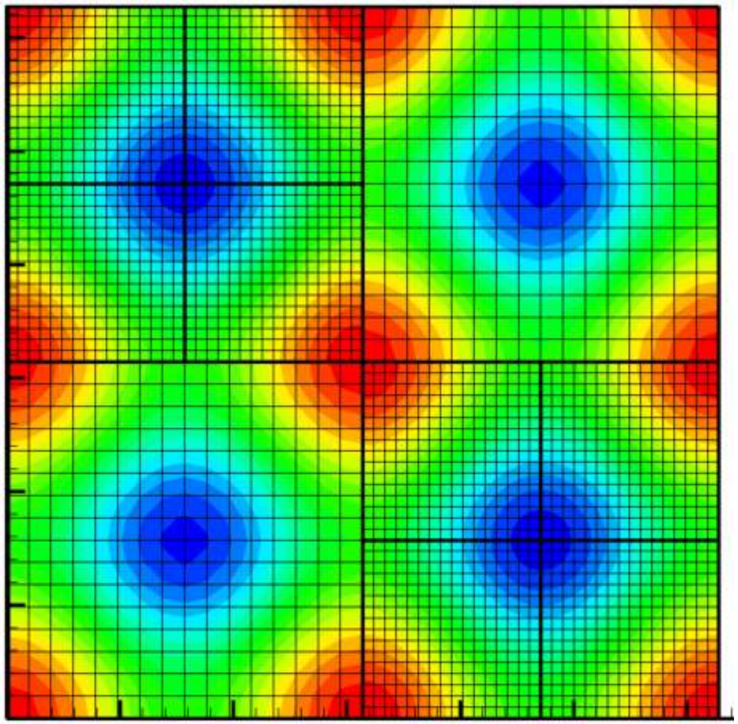
Validation: Taylor Green Vortex

- Compare numerical solution to analytical solution of 2D Navier-Stokes equations
- Domain:
  [π/2, 5π/2]x [π/2, 5π/2]
- Homogeneous Dirichlet/Neumann velocity boundary conditions and Neumann pressure boundary condition

$$u = -e^{-2t} \cos x \sin y$$

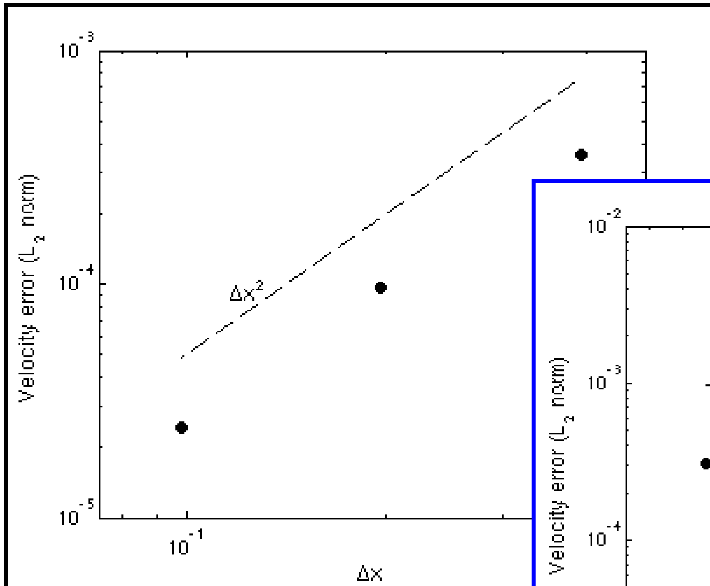
$$v = e^{-2t} \sin x \cos y$$

$$p = -\frac{e^{-4t}}{4} (\cos 2x + \cos 2y)$$



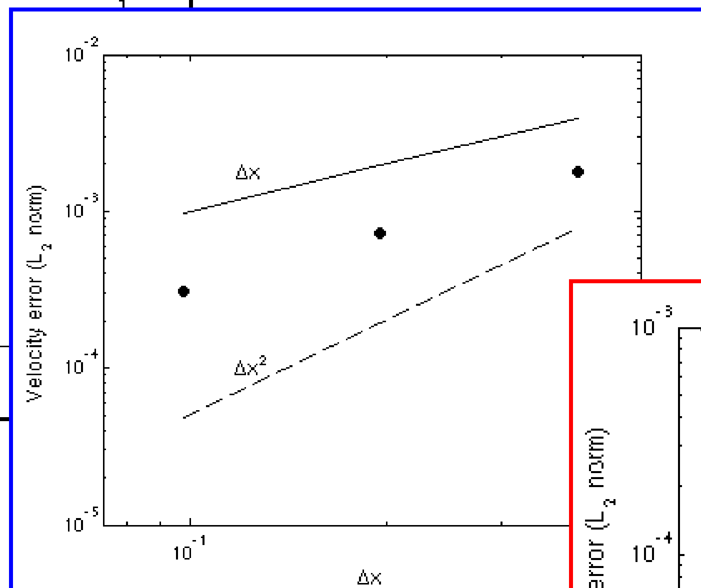
Adaptive mesh refinement: accuracy

Validation: Taylor Green Vortex, no temporal AMR

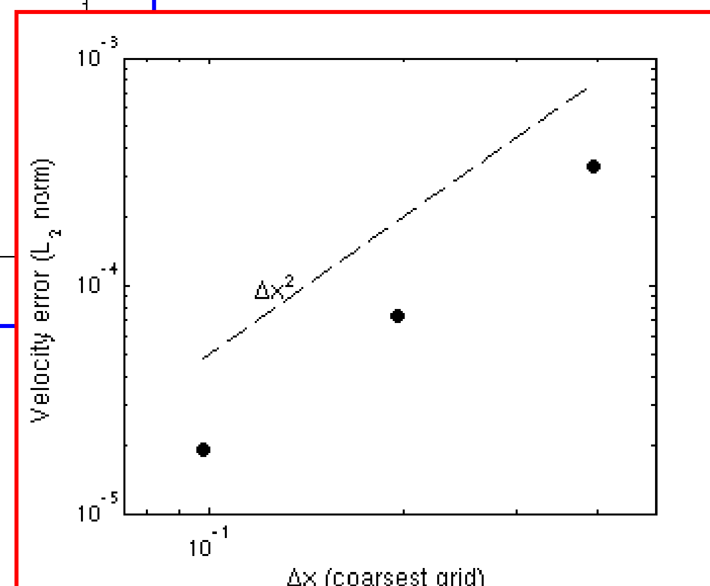


Uniform domain

Domain with 2 refinement levels
Linear interpolation

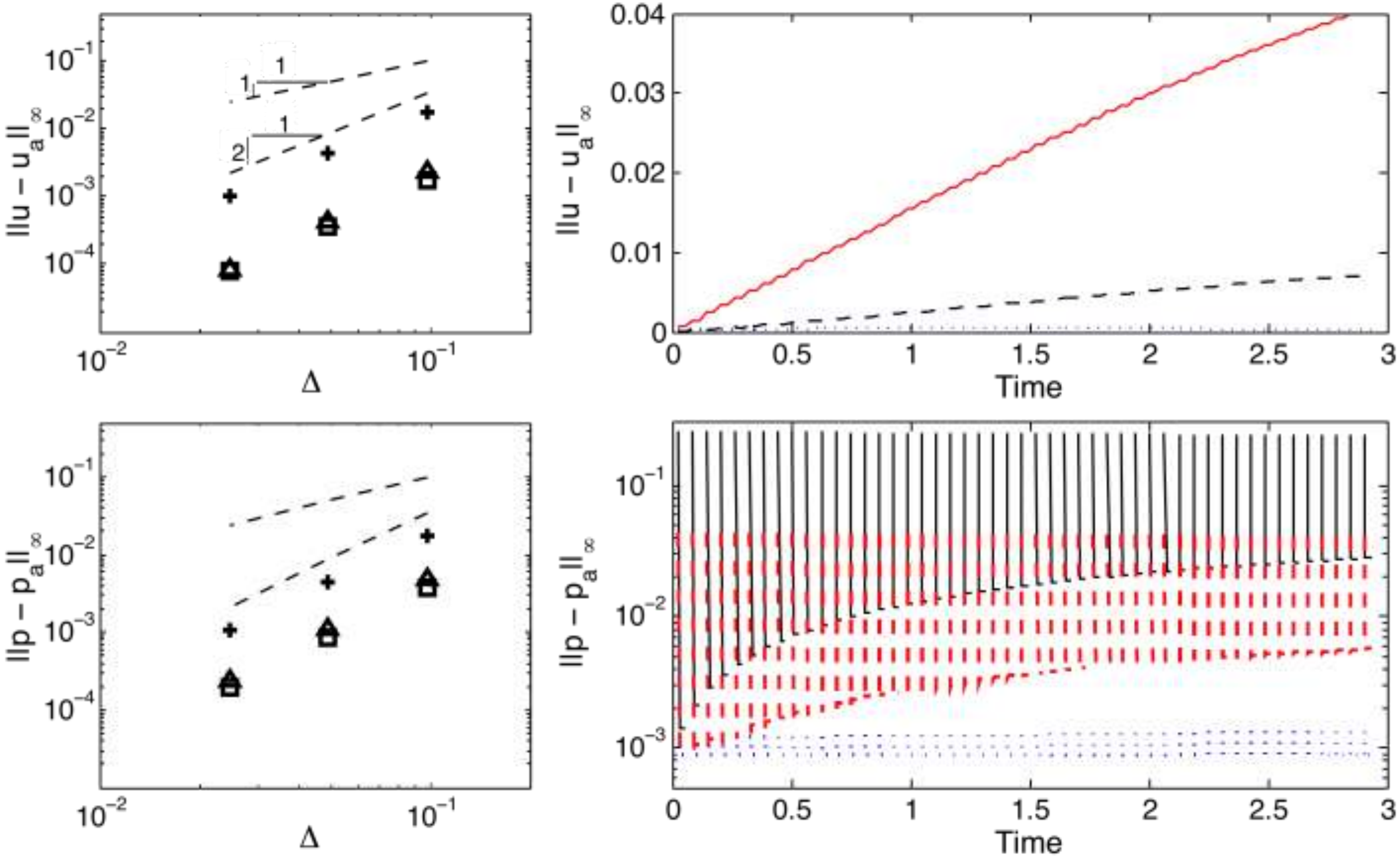


Domain with 2 refinement levels
Quadratic interpolation



Adaptive mesh refinement: accuracy

Validation: Taylor Green Vortex, with temporal AMR*

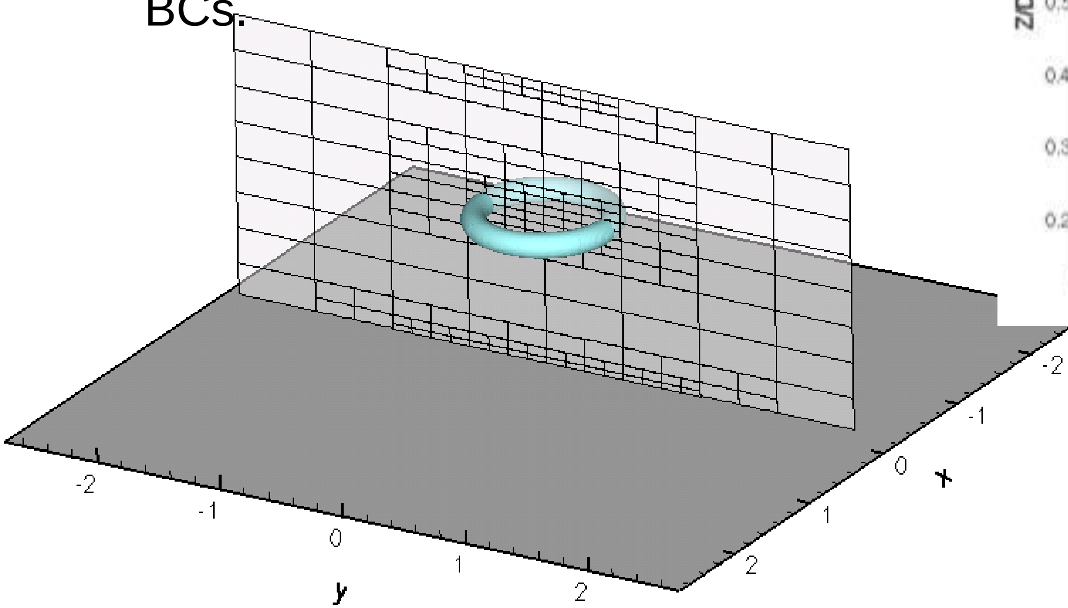


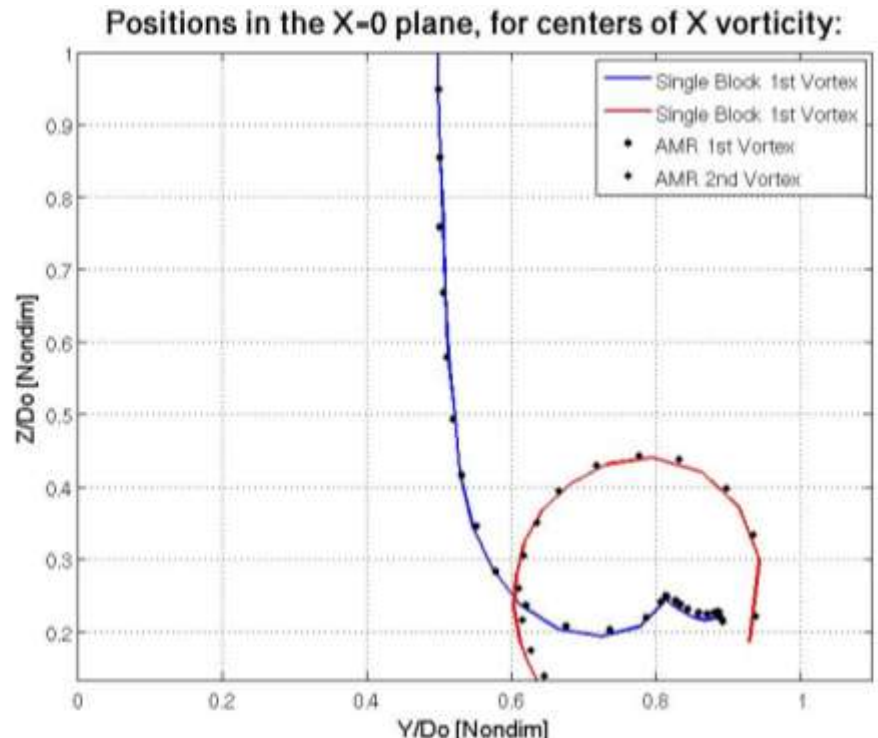
Vanella & Balaras, J. Comput. Physics, 2010

Adaptive mesh refinement: validation

Vortex Ring impinging on a wall, Re ≈ 570

- Compare AMR solution to numerical solution using a Single Block, Cartesian solver.
- Velocity Dirichlet BCs in top and Bottom Boundaries, periodic on side walls. Pressure Neumann BCs.





Q contour for vortex impinging normal to a wall, Re ≈ 570

Adaptive mesh refinement: validation

Vortex Ring impinging on a wall, Re ≈ 570

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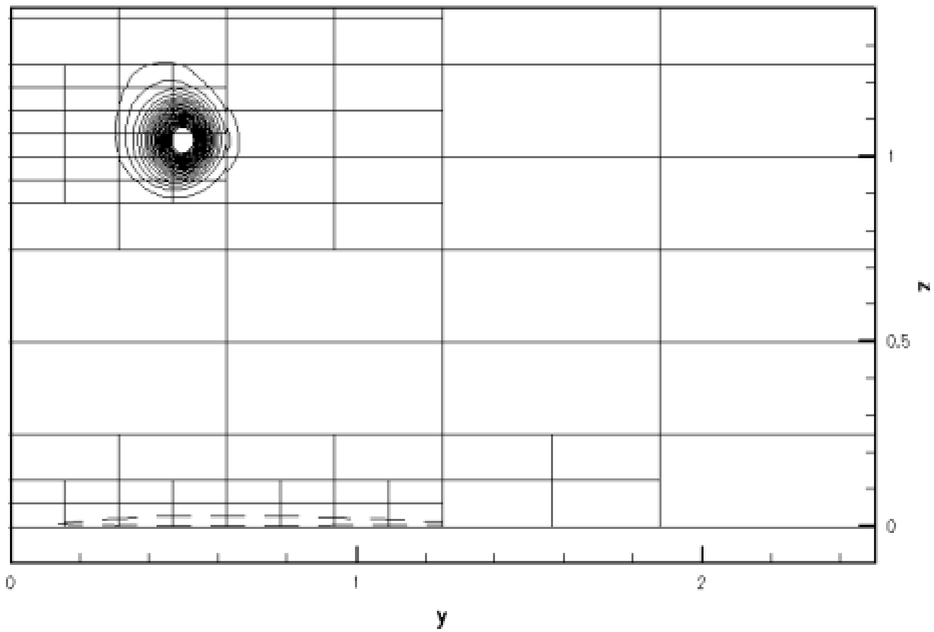
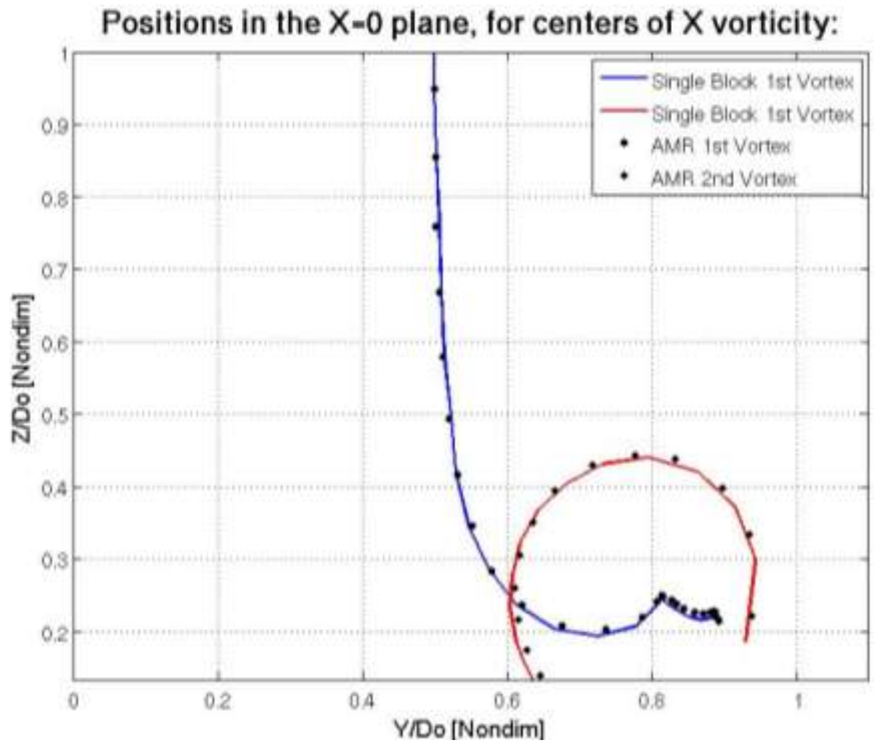
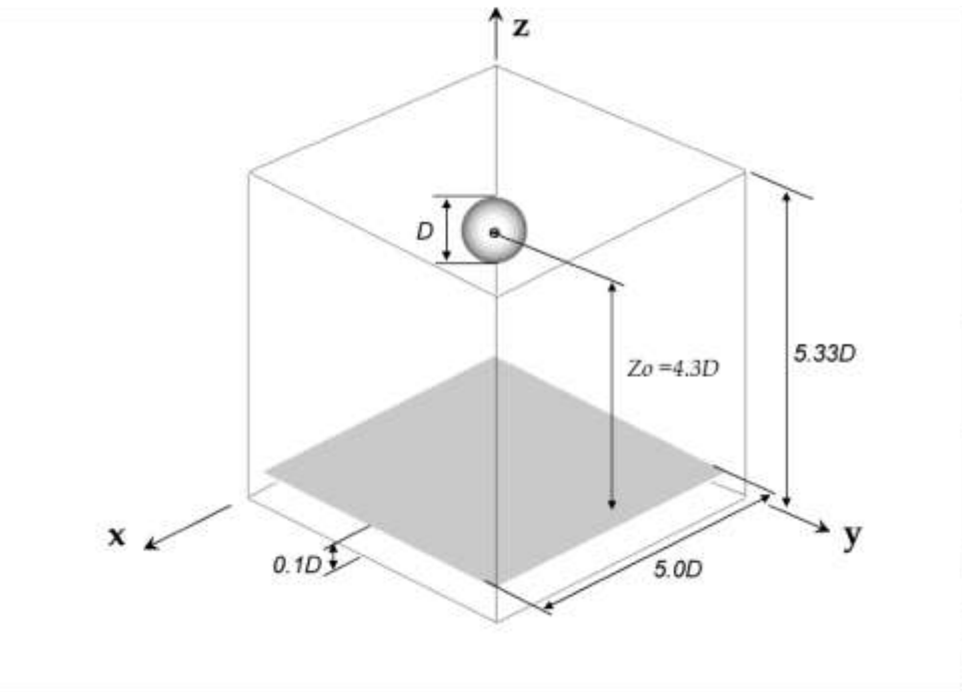


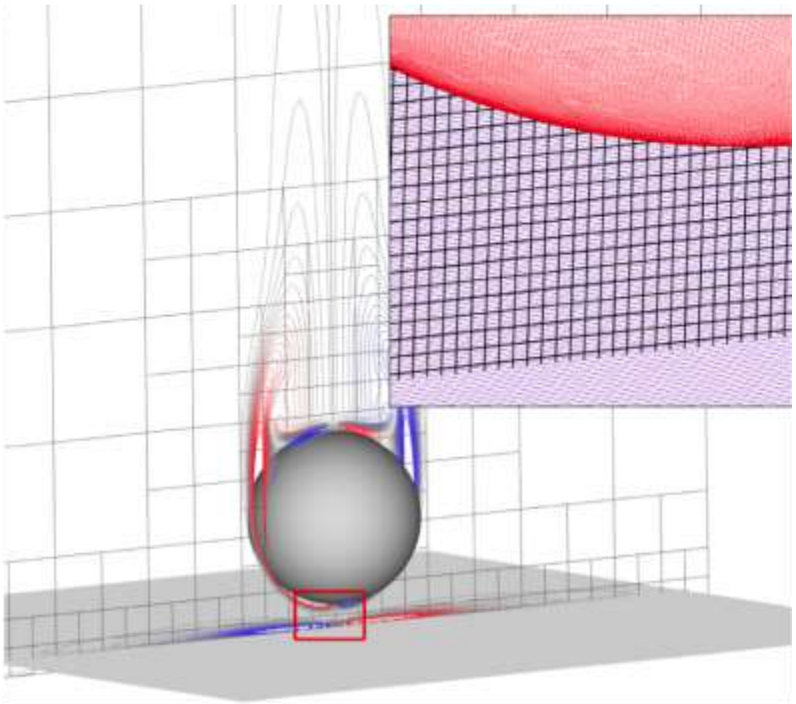
vorticity isolines at a cross section, Re ≈ 570



Sphere bouncing-off a wall



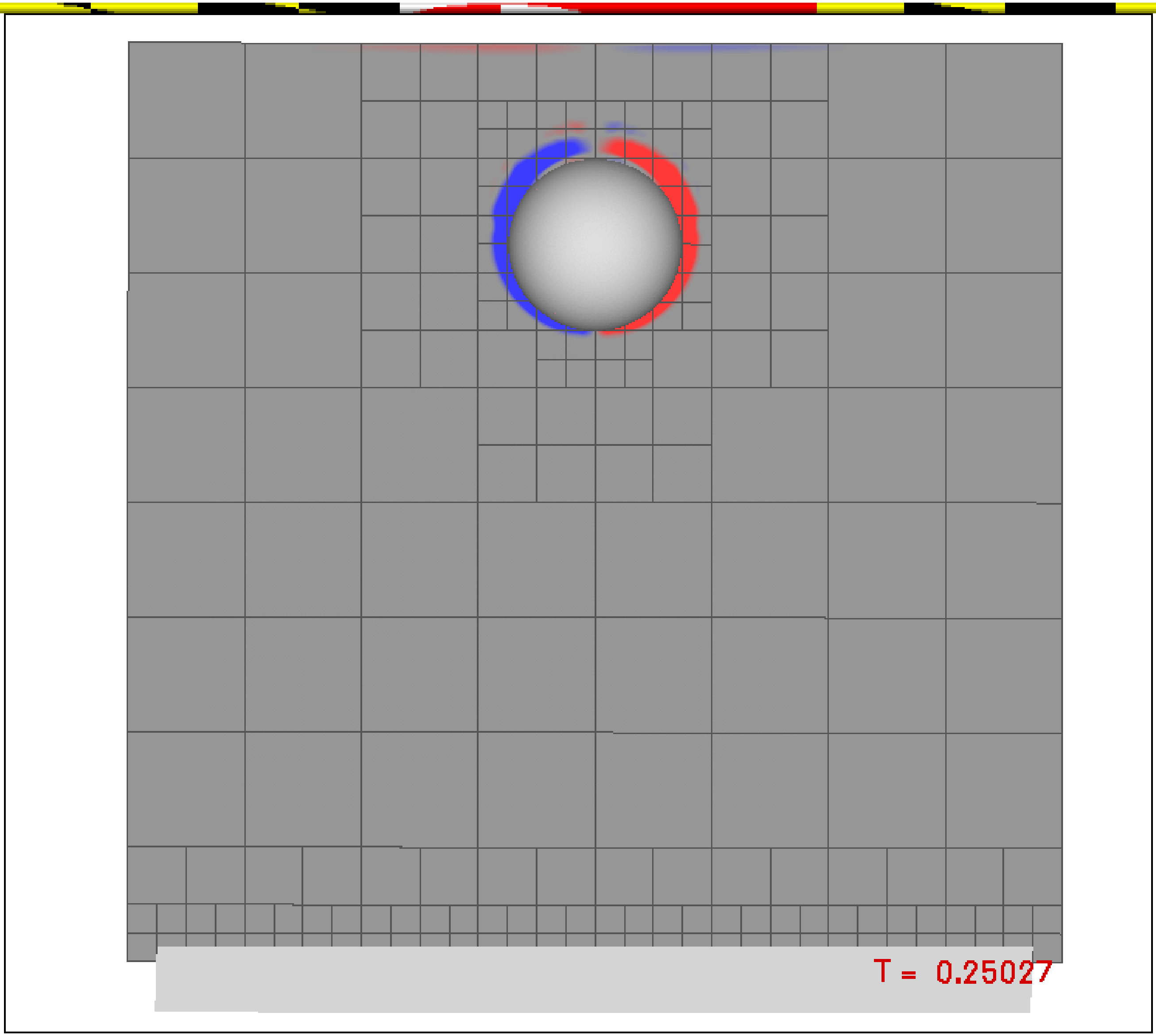
(a)



(b)

Computational setup and Eulerian/Largangian grid arangement

Sphere bouncing-off a wall



Dry restitution coefficient one

Parallel AMR solver: LES module

Critical issues with AMR/LES:

- In DNS and RANS, the solution is smooth on the grid scale and interpolation errors due to the reconstruction of the fluxes at the non matching interfaces between coarse and fine grids are small.

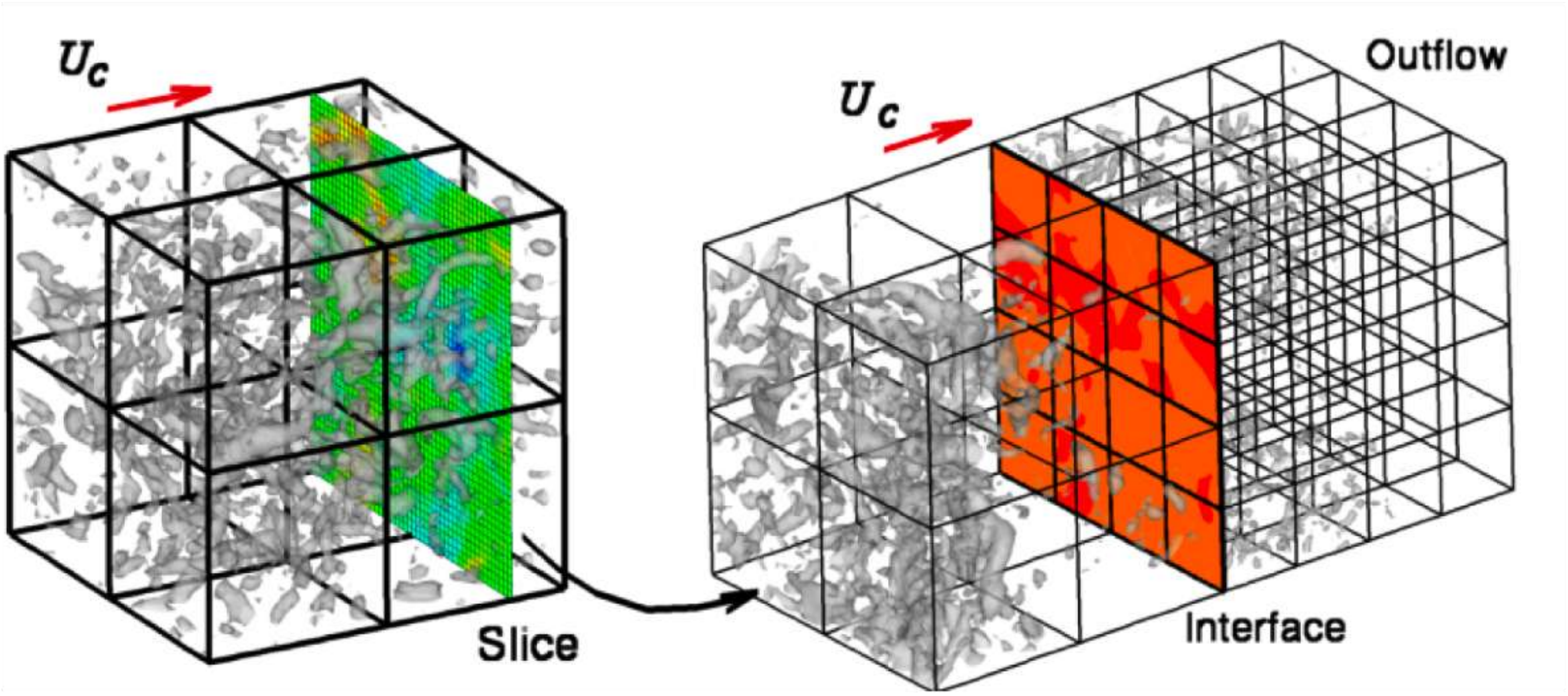
- In LES the flow is not smooth at the smallest scale and numerical errors in the interpolation between grids can be significant.

- The subgrid-scale (SGS) eddy viscosity is usually proportional to the filter width squared. A sudden mesh refinement or coarsening results in a discontinuity in eddy viscosity.

- When a non-uniform filter width is used, differentiation and filtering do not commute, and additional terms ("commutator errors") appear in the equations of motion.

Parallel AMR solver: LES module

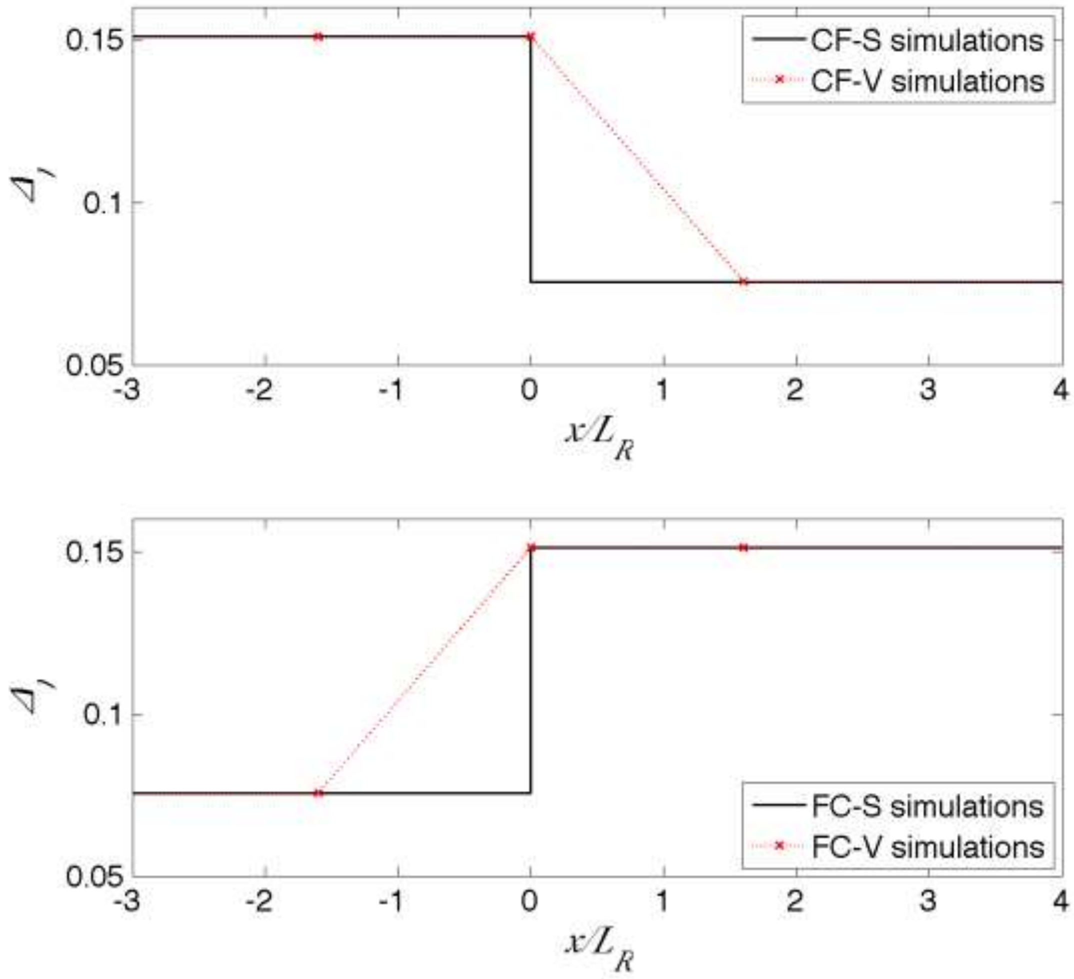
Homogeneous turbulence convected through a CF interface:



Vanella & et. al., J. Turbulence, 2008

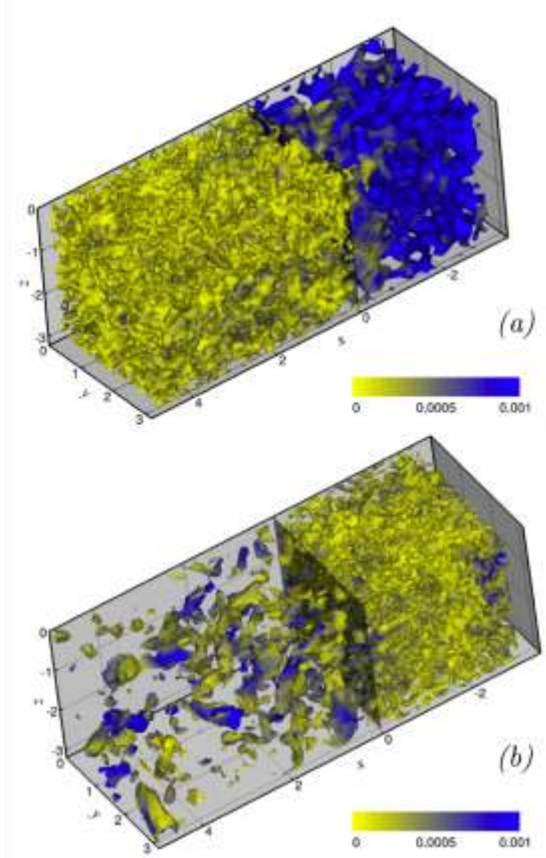
Parallel AMR solver: LES module

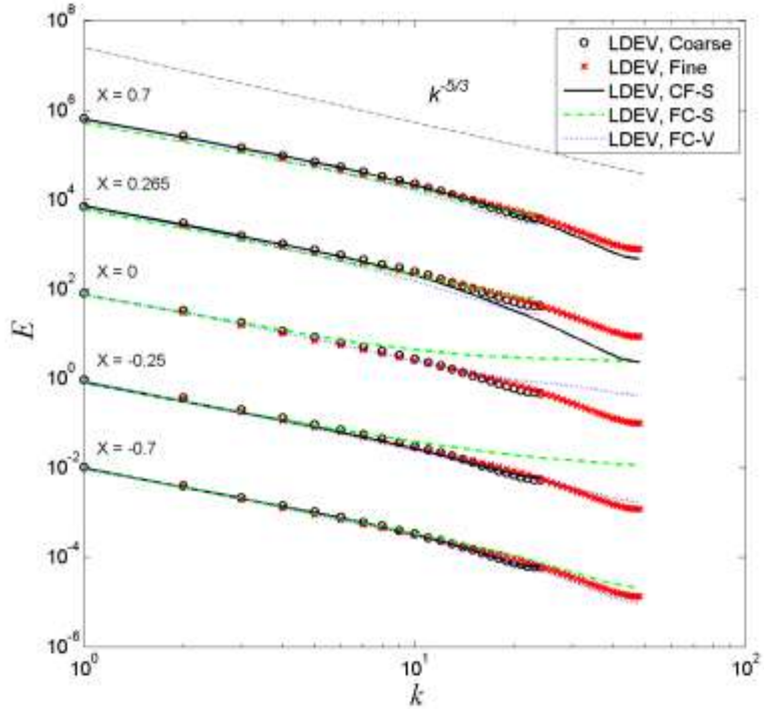
Filter size near the interface:

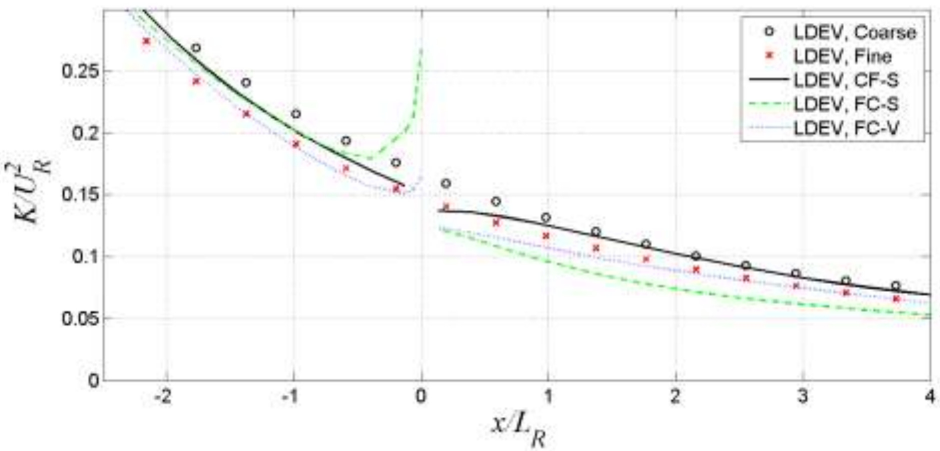


Parallel AMR solver: LES module

Effects of filter size

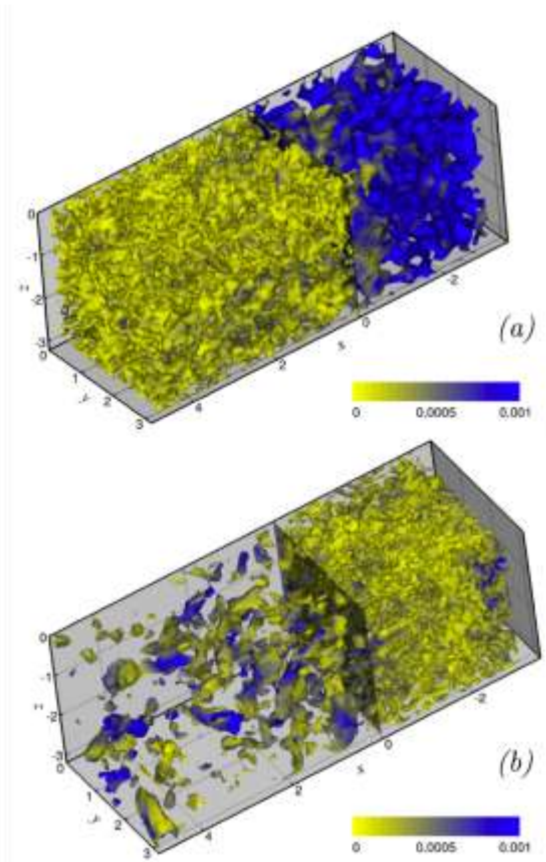


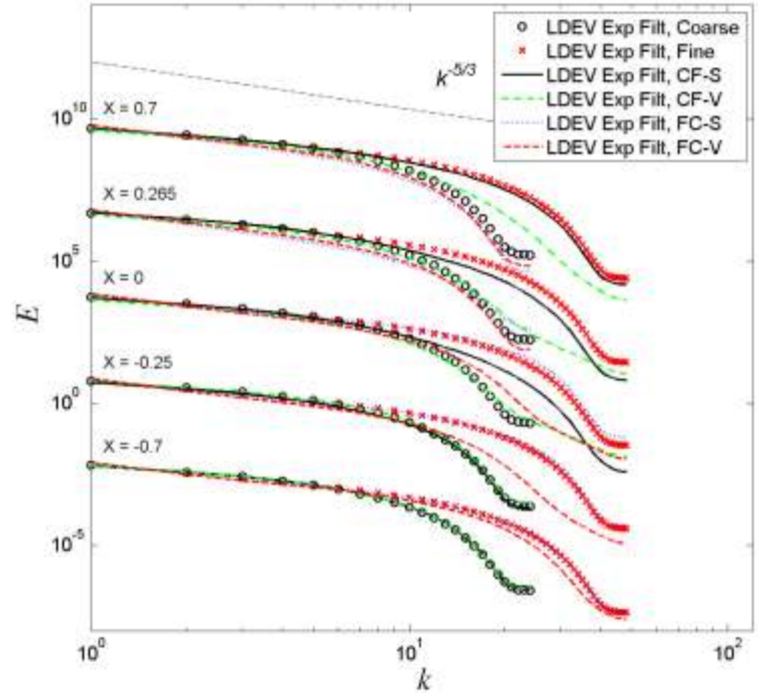


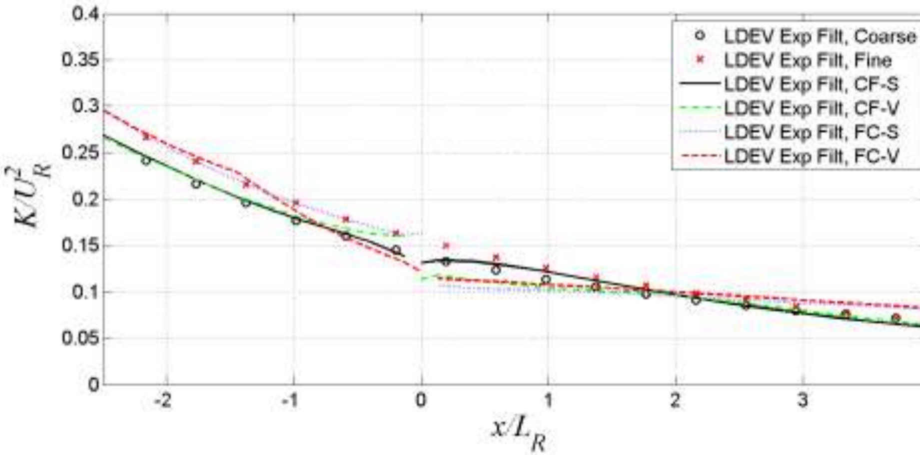


Parallel AMR solver: LES module

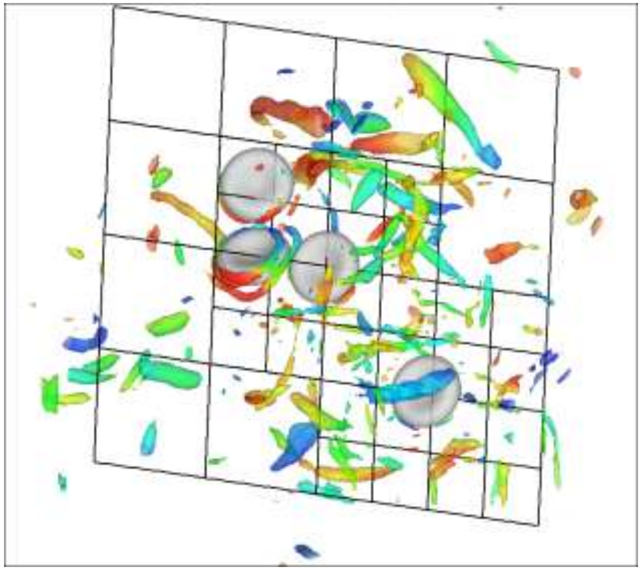
Effects of explicit filtering

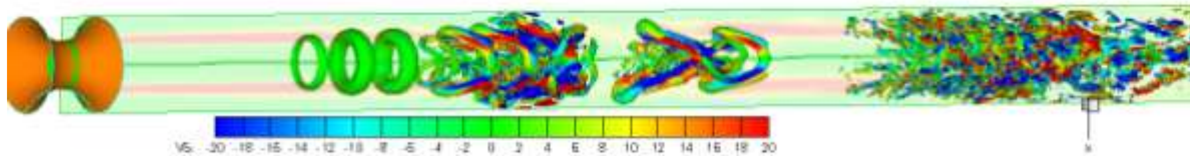


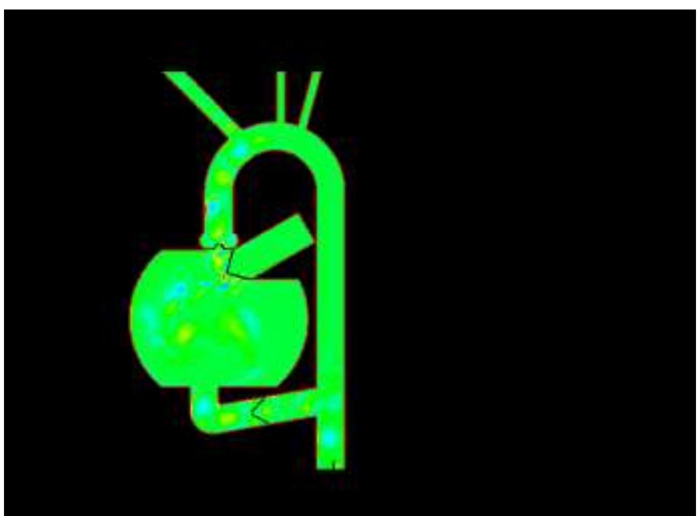


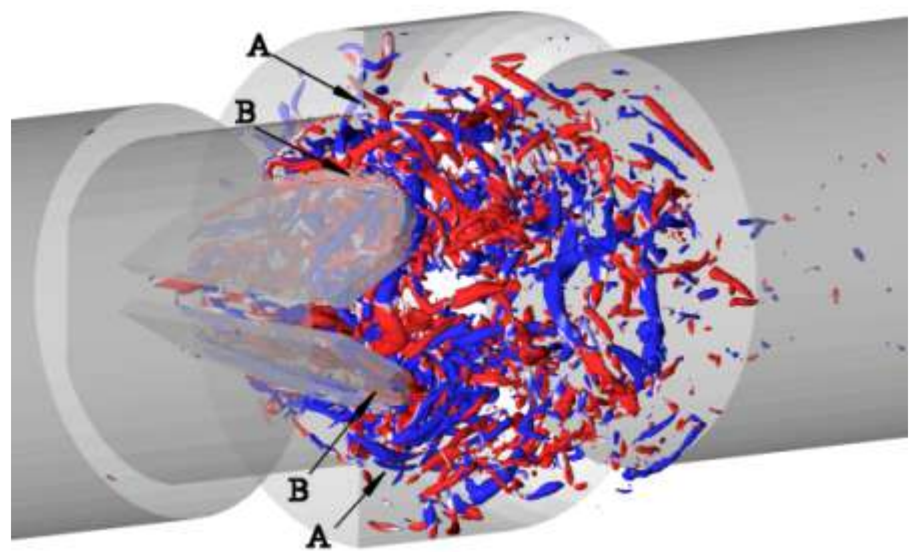


Applications

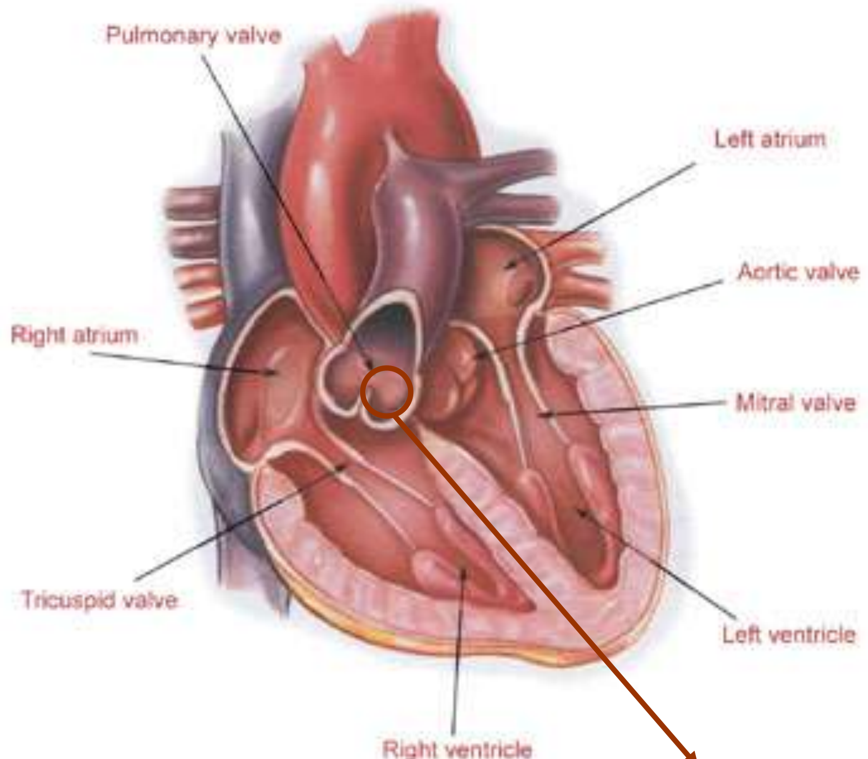








Example: Heart valve disease and treatment



CALCIFIED AORTIC VALVE

- 4 chambers
  - 2 atriums
  - 2 ventricles
- 4 valves
  - 2 atrioventricular
  - 2 semilunar
- Left side; high pressure
- Right side: low pressure
- Mitrial and Aortic valves are the most commonly affected valves

Example: Heart valve disease and treatment

- Valvular Heart Disease:
  - Not regarded as major public health problem?
  - Common and Underdiagnosed?

Burden of valvular heart diseases: a population-based study

Vuyisile T Nkomo, Julius M Gardin, Thomas N Skelton, John S Gottdiener, Christopher G Scott, Maurice Enriquez-Sarano

Background Valvular heart diseases are not usually regarded as a major public-health problem. Our aim was to assess their prevalence and effect on overall survival in the general population.

Methods We pooled population-based studies to obtain data for 11 911 randomly selected adults from the general population who had been assessed prospectively with echocardiography. We also analysed data from a community study of 16 501 adults who had been assessed by clinically indicated echocardiography.

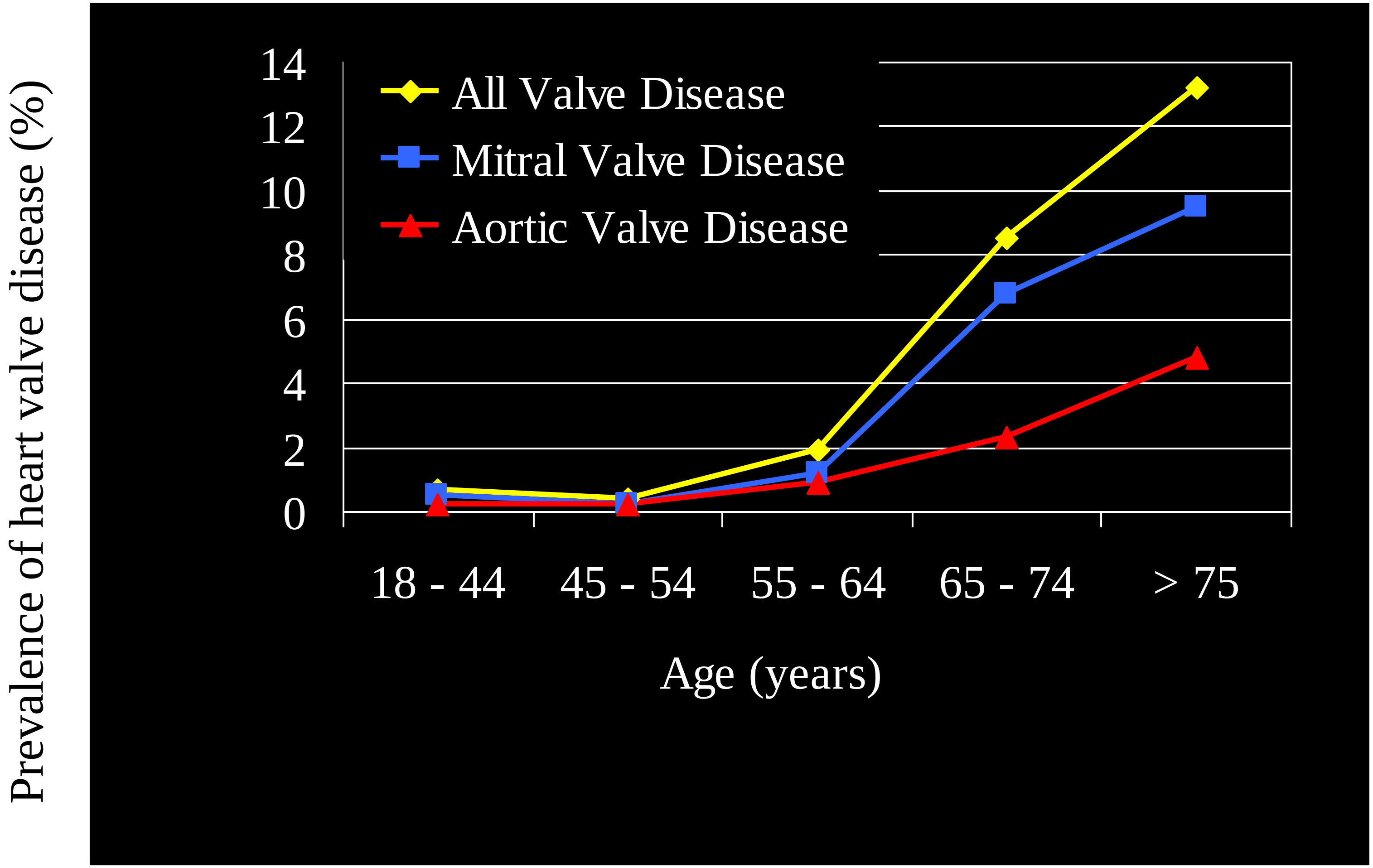
Lancet 2006; 368: 1005–11

Published Online August 18, 2006 DOI:10.1016/S0140-6736(06)69208-8

See Comment page 969

Mayo Clinic, Rochester, MN,

Example: Heart valve disease and treatment



Nkomo VT et al. Burden of valvular heart diseases: a population-based study
Lancet 2006; 368:1005-11

Example: Heart valve disease and treatment

- Replacement of defective heart valves with artificial prostheses is a ‘safe’ and routine surgical procedure worldwide
- 12% of adults over 70 will has mitral or aortic valve disease.
- Several different types of prosthetic valves:
  - Mechanical HV
  - Bioprosthetic (tissue) HV
- Prosthetic valves **cannot** exactly mimic natural valves
- Thrombogenesis is a major complication (2% year)
- Developing new designs is expensive and time consuming:
  - In-vitro testing / animal studies / clinical trials
  - Takes more than 10 years and ~$50 million
- Predictive computer simulations can reduce cost

Example: Heart valve disease and treatment

Long-term results with conventional AVR: Bad for the Brain

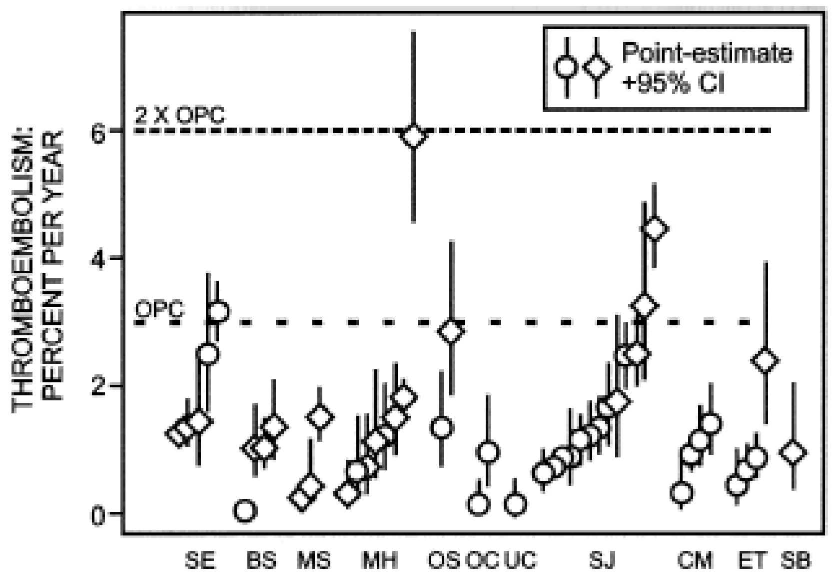
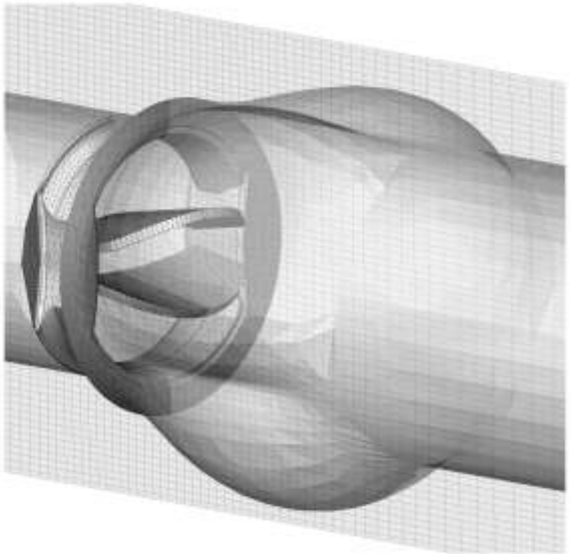
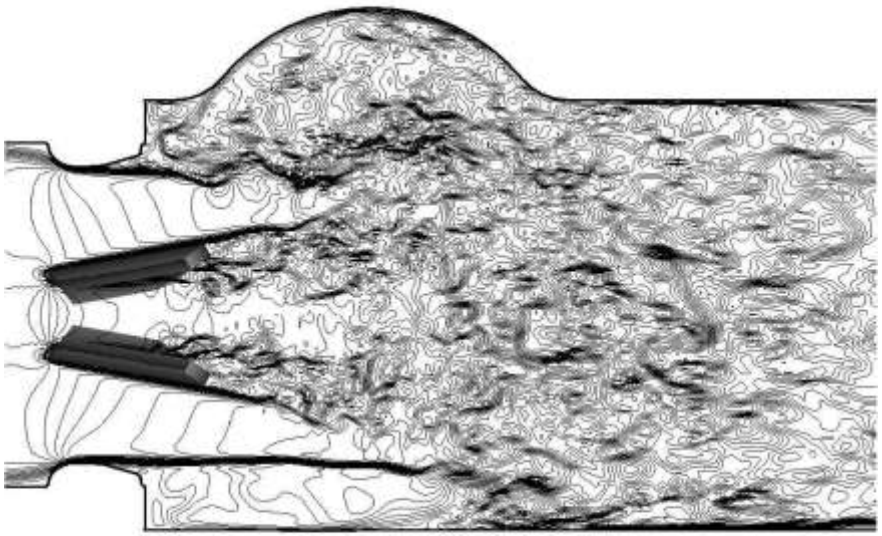
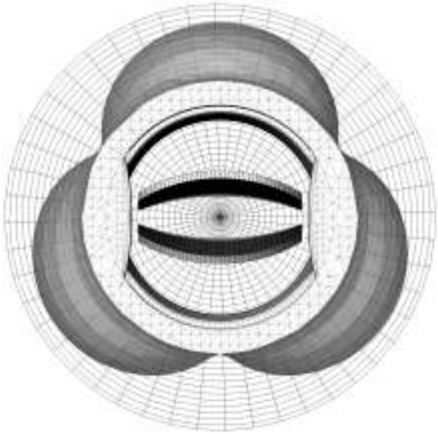


Figure 3. Thromboembolism rates for mechanical aortic valves. The vertical axis is the linearized rate in percentage per year. Each symbol represents one series. Circles indicate that only late events were used to calculate the rates; diamonds indicate that both early and late events were used. BS = Bjork Shiley; CM = Carbomedics; ET = Edwards Tekna or Duromedics; MH = Medtronic Hall; MS = Monostrut; OC = Omnicarbon; OPC = FDA's Objective Performance Criteria (from reference 29); OS = Omniscience; SB = Sorbin Bicarbon; SE = Starr Edwards; SJ = St. Jude; UC = Ultracor. From reference 29.

Level 1: Assessment of PHV performance through hydrodynamic modeling*







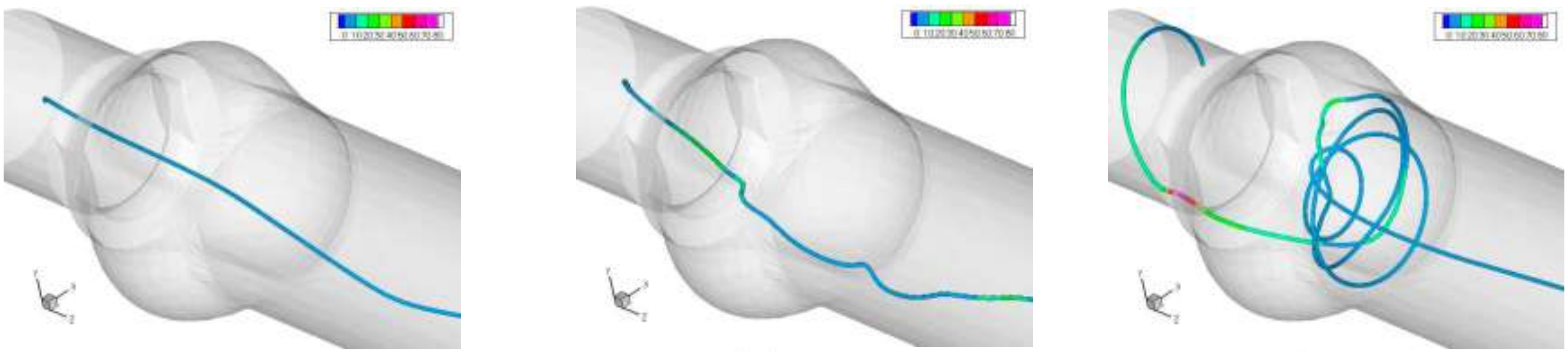
- Direct numerical simulation of the fluid structure interaction problem (solution of NS equations, Newtonian fluid, incompressible flow.
- Detailed information macroscopic flow patterns

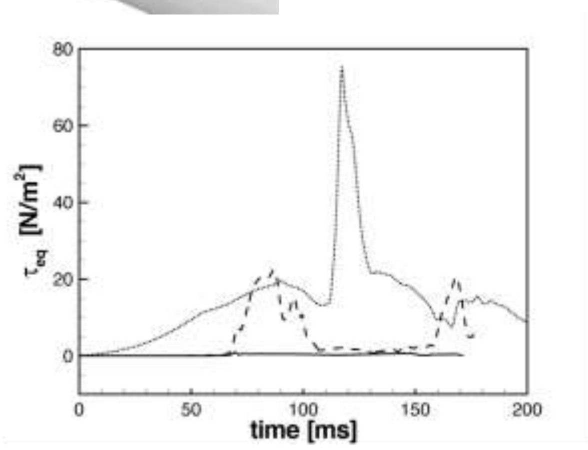
*DeTulio et. al. J. Fluid Mech. (2009)

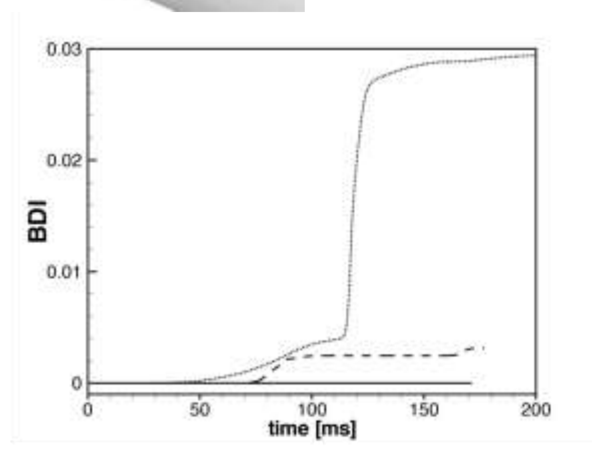
Example: Heart valve disease and treatment

Level 2: Hemolysis and thrombosis modeling

- Mechanical hemolysis is the result of excessive hydrodynamic forces on the red blood cell's (RBC) membrane.
- Frequently used models relates hemolysis levels to the stress scalar magnitude and duration of exposure, based on data coming from steady shear experiments at short time scales.







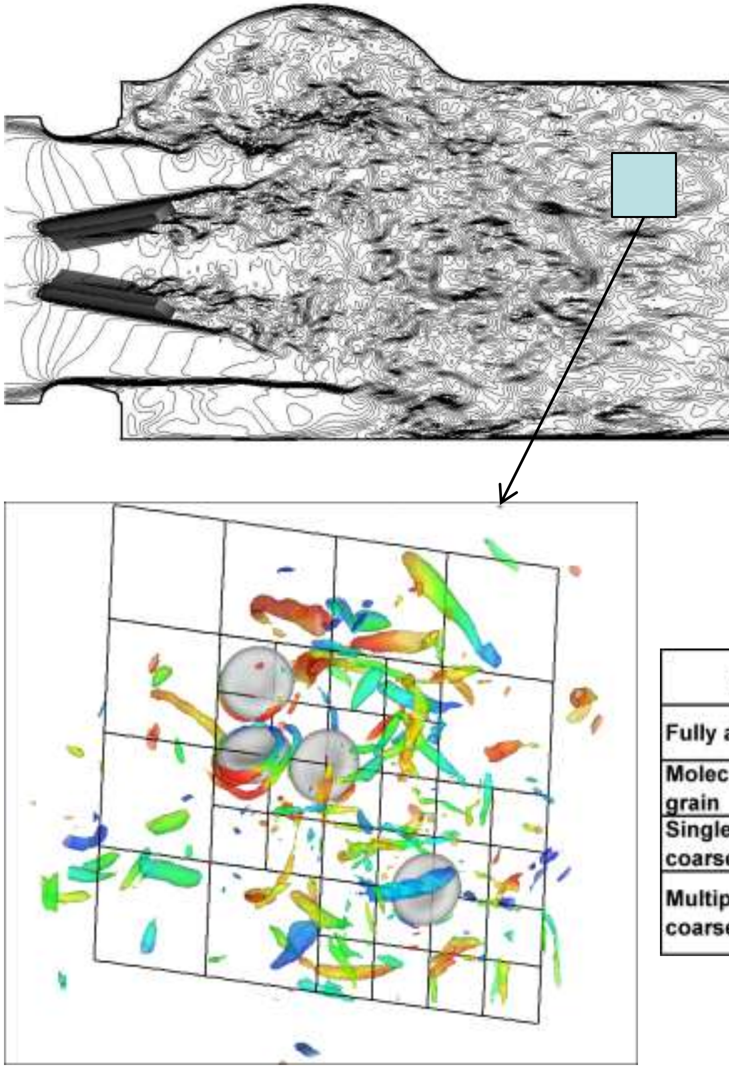
Example: Heart valve disease and treatment

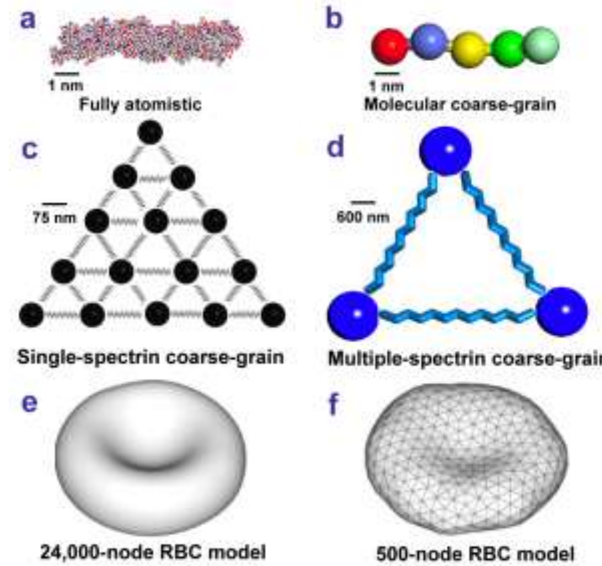
Level 2: Hemolysis and thrombosis modeling current limitations

- Important questions need to be addressed:
  - How important is the local history of stress exposure (i.e. successive application of high stress fields) to determining the effective hemolysis limits?
  - What is the effect of neighboring cells in the suspension on mitigating or amplifying the effective stress on the cell?

Example: Heart valve disease and treatment

Level 3: Developing better hemolysis and thrombosis models through whole blood simulations





Model	RBC structure	Particles per RBC	Force field parameters	Fluid structure	RBCs per simulation
Fully atomistic	Bonded atoms	10^{10} - 10^{11}	100	Atomistic	<< 1 (one protein network unit cell)
Molecular coarse grain	Bonded multi-atom beads	10^{6} - 10^{8}	20	Multi-atom beads or continuum	1 - 10
Single-spectrin coarse-grain	Nodes joined by spectrin links	10^{4}	10	Continuum	1,000
Multiple-spectrin coarse-grain	Pseudo-nodes joined by pseudo-spectrin links	$< 10^{3}$	10	Continuum	1,000,000

Example: Heart valve disease and treatment

Level 3: whole blood simulations on Petascale computing platforms

- Sample computation:
  - 3 million blocks (32^3)
  - 5 million blood elements (1000 degrees of freedom each)
  - 10^4 timesteps
  - 16 million hours, wall clock on 100k cores is 6.6 days
  - data to be stored: 1.2 Pbytes

- Challenges:
  - Explore fine grain parallelism due to the large number of cores $O(10^5)$
  - Utilize MPI and direct p-threads