

On forward in time differencing: an unstructured mesh framework

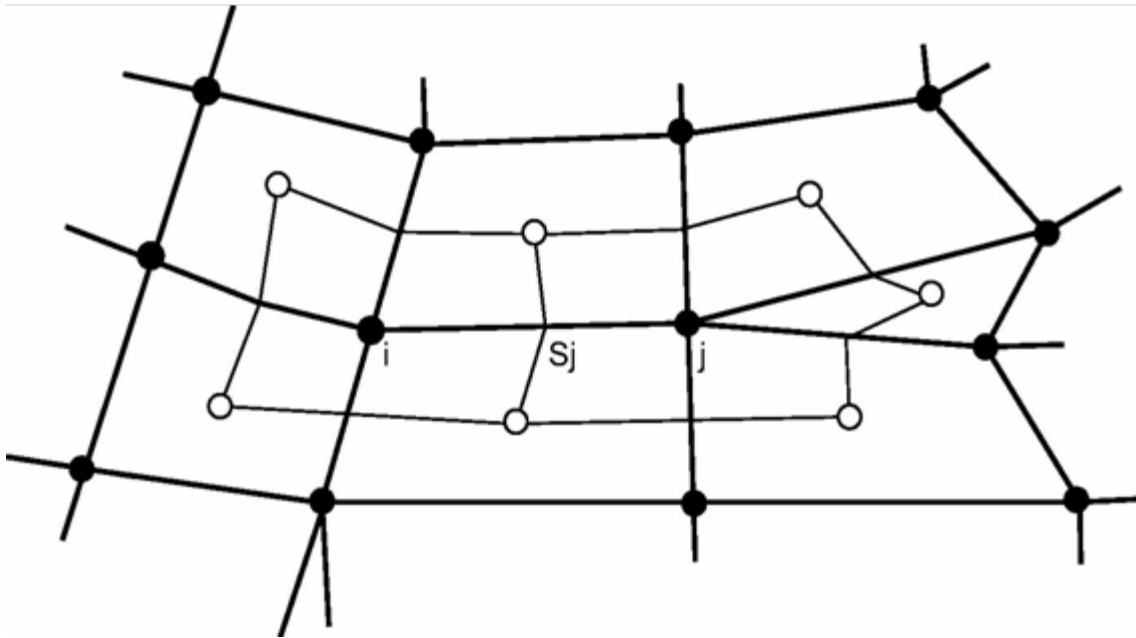
Joanna Szmelter
Loughborough University
UK

Piotr Smolarkiewicz
NCAR
Colorado USA

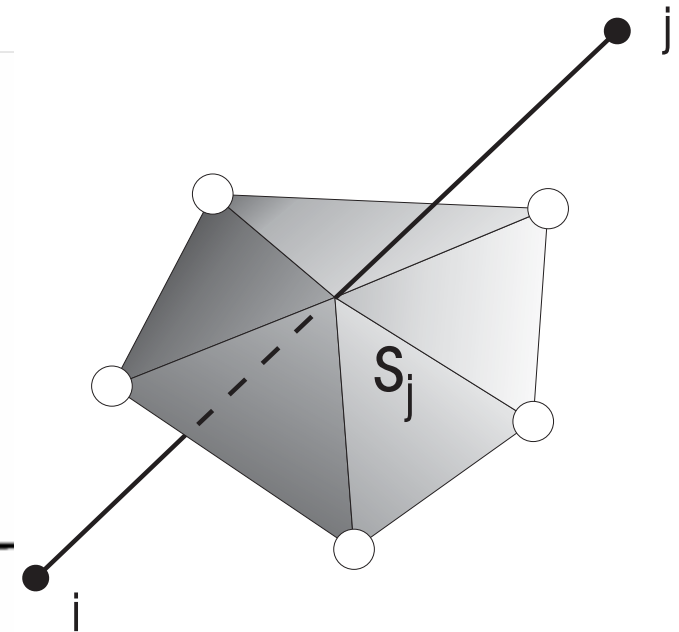
Edge based data *Finite Volume*

(Smolarkiewicz, Szmelter JCP 2005)

2D

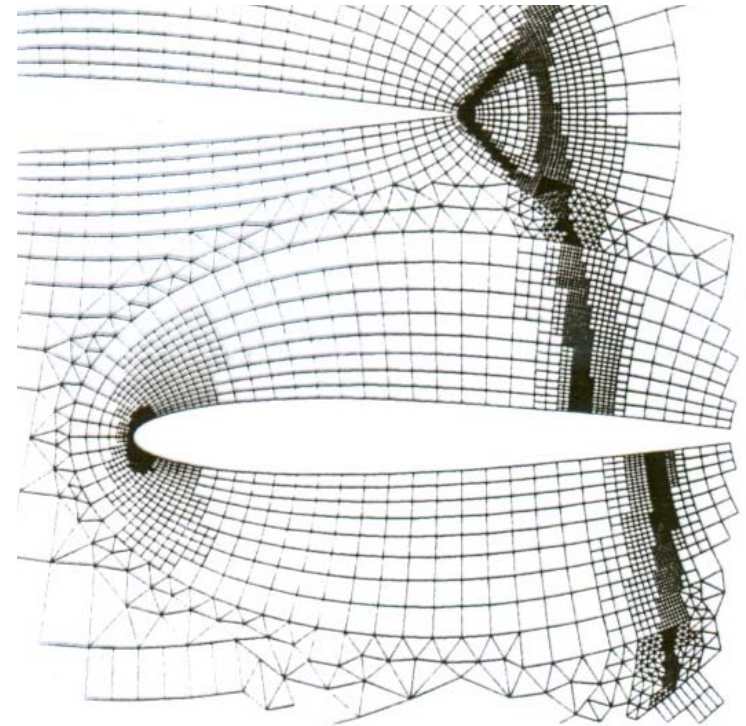


3D

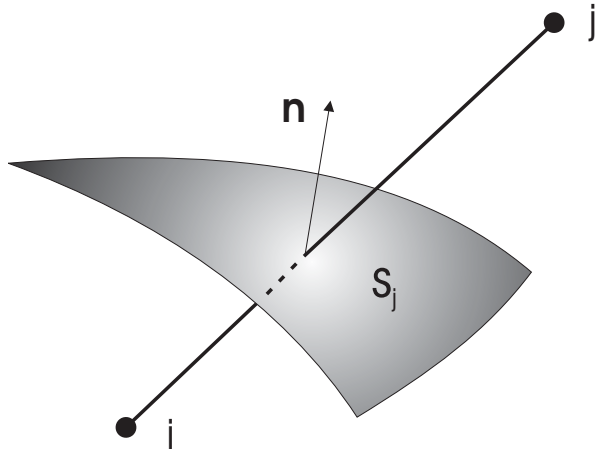


Edge based data structure

- ☺ *Flexible mesh adaptivity and hybrid meshes*
- ☺ *Low storage*
- ☺ *Easy generalisation to 3D, vectorisation, parallelisation, mesh agglomeration*
- ☺ *Less expensive than element based data structure*
- ☹ *More expensive operations than I,J,K*



Notion of the edge-based MPDATA: ADVECTION



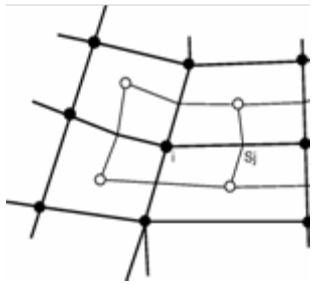
$$\frac{\partial \Psi}{\partial t} = -\nabla \cdot (\mathbf{v}\Psi)$$

$$\Psi_i^{n+1} = \Psi_i^n - \frac{\delta t}{\mathcal{V}_i} \sum_{j=1}^{l(i)} F_j^\perp S_j$$

$$F_j^\perp = [v_j^\perp]^+ \Psi_i^n + [v_j^\perp]^- \Psi_j^n$$

*FIRST ORDER UPWIND
(DONOR CELL)*

$$[v]^\perp := 0.5(v + |v|) \quad , \quad [v]^\perp := 0.5(v - |v|)$$



$$F_j^\perp = v_j^\perp \Psi|_{s_j}^{n+1/2} + \text{Error}$$

$$\tilde{v} := -\frac{1}{\Psi} \text{Error}$$

compensating velocity

$$\begin{aligned} \text{Error} = & -0.5|v_j^\perp| \left. \frac{\partial \Psi}{\partial r} \right|_{s_j}^* (r_j - r_i) + \boxed{0.5v_j^\perp \left. \frac{\partial \Psi}{\partial r} \right|_{s_j}^* (r_i - 2r_{s_j} + r_j)} \\ & + 0.5\delta t v_j^\perp (\mathbf{v}\nabla\Psi)|_{s_j}^* + 0.5\delta t v_j^\perp (\Psi\nabla\cdot\mathbf{v})|_{s_j}^* + \mathcal{O}(\delta r^2, \delta t^2, \delta t\delta r) \end{aligned}$$

MPDATA BASIC SCHEME

ITERATED UPWIND

- Calculate normal velocity v_j^\perp
- Calculate fluxes

$$F_j^\perp = [v_j^\perp]^+ \Psi_i^n + [v_j^\perp]^- \Psi_j^n$$

- Update field

$$\Psi_i^* = \Psi_i^n - \frac{\delta t}{\mathcal{V}_i} \sum_{j=1}^{l(i)} F_j^\perp$$

- Calculate antidiffusive pseudo velocity

$$\hat{v}_j^\perp = |v_j^\perp| \frac{|\Psi_j^*| - |\Psi_i^*|}{|\Psi_j^*| + |\Psi_i^*| + \varepsilon} - \frac{\delta t}{2} v_j^\perp \left(\mathbf{v} \cdot \frac{\nabla |\Psi^*|}{|\Psi^*|} + \nabla \cdot \mathbf{v} \right)_{S_j}$$

- Calculate fluxes

$$F_j^* = [\hat{v}_j^\perp]^+ \Psi_i^* + [\hat{v}_j^\perp]^- \Psi_j^*$$

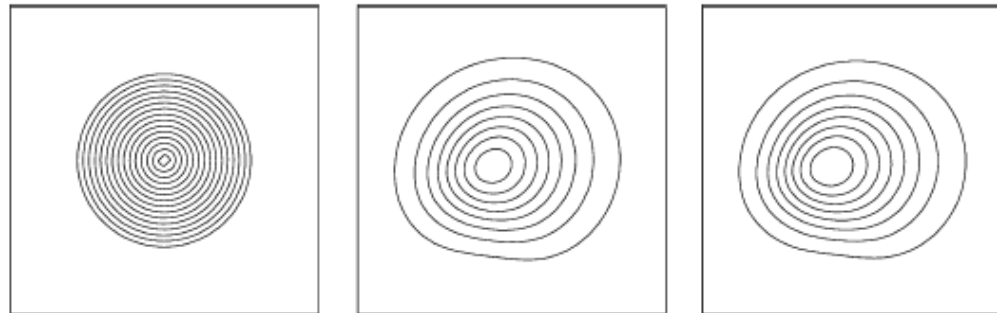
- Update field

$$\tilde{\Psi}_i^{n+1} = \tilde{\Psi}_i^* - \frac{\delta t}{\mathcal{V}_i} \sum_{j=1}^{l(i)} F_j^*$$

FIRST ORDER UPWIND

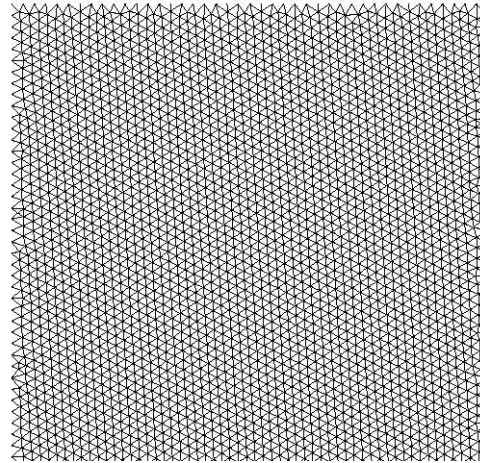
FIRST ORDER UPWIND

Structured v Unstructured



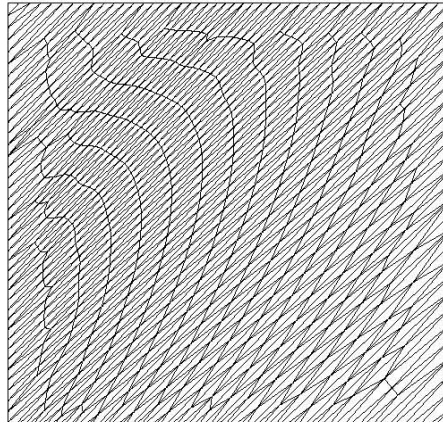
Scheme	Max	Min	L_∞	L_2
MPDATA FD	2.18	0.	2.00	0.47×10^{-3}
MPDATA FV squares	2.18	0.	2.00	0.47×10^{-3}
MPDATA FV triangles, $\delta t = 0.1$	2.19	0.	1.92	0.47×10^{-3}
MPDATA FV triangles, $\delta t = 0.061$	2.08	0.	2.09	0.52×10^{-3}
Upwind FD	0.27	0.	3.76	1.21×10^{-3}
Upwind FV squares	0.28	0.	3.76	1.04×10^{-3}
Upwind FV triangles	0.25	0.	3.68	1.06×10^{-3}
Leapfrog FD	3.16	-0.62	1.68	0.62×10^{-3}
Leapfrog FV squares	3.11	-0.67	1.71	0.64×10^{-3}
Leapfrog FV triangles	3.11	-0.69	1.74	0.65×10^{-3}

CONVERGENCE OF FINITE-VOLUME MPDATA ON UNSTRUCTURED MESH



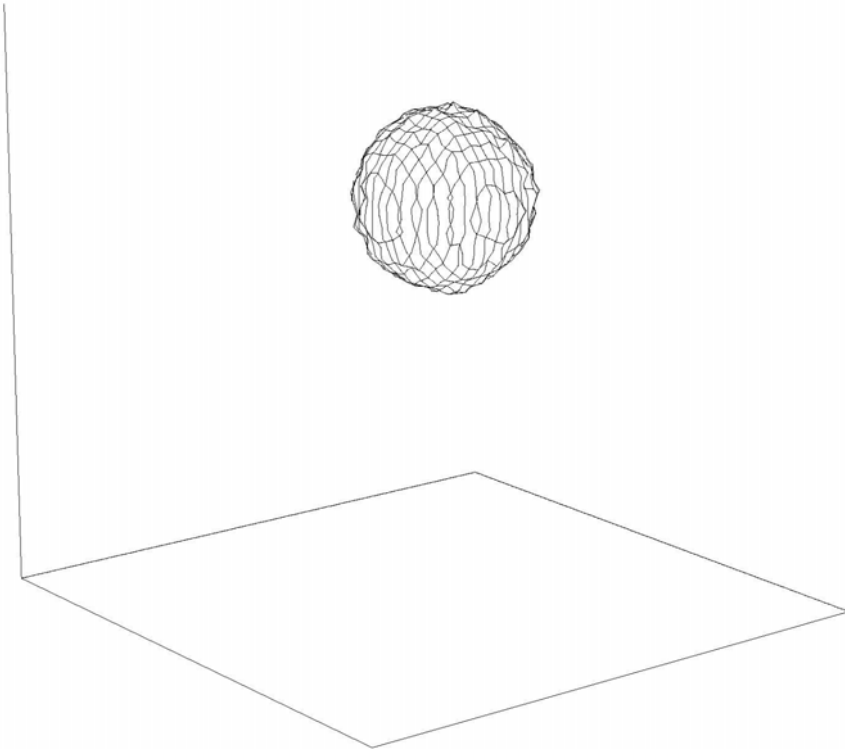
background spacing	L_∞	L_2	L_1
2.00	$2.95 \cdot 10^{-2}$	$8.73 \cdot 10^{-3}$	$1.83 \cdot 10^{-3}$
1.00	$7.69 \cdot 10^{-3}$	$2.22 \cdot 10^{-3}$	$4.73 \cdot 10^{-4}$
0.50	$1.93 \cdot 10^{-3}$	$5.57 \cdot 10^{-4}$	$1.19 \cdot 10^{-4}$
0.25	$4.86 \cdot 10^{-4}$	$1.43 \cdot 10^{-4}$	$3.07 \cdot 10^{-5}$

CONVERGENCE OF FINITE-VOLUME MPDATA ON UNSTRUCTURED SKEWED MESH

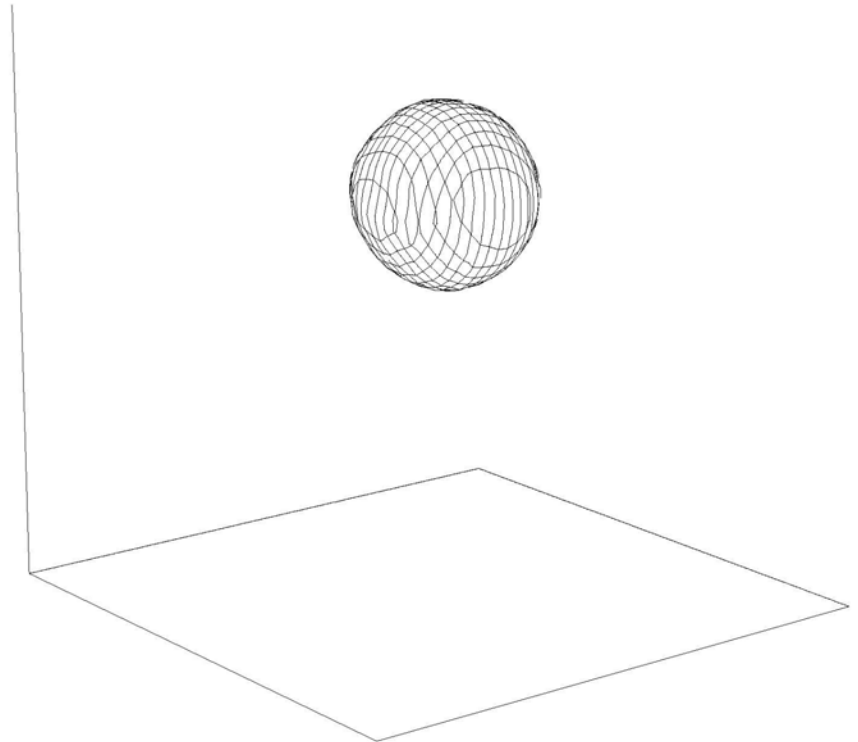


δ_E	L_∞	L_2	L_1
3.99	$3.58 \cdot 10^{-1}$	$1.38 \cdot 10^{-1}$	$2.86 \cdot 10^{-2}$
2.05	$2.01 \cdot 10^{-1}$	$6.68 \cdot 10^{-2}$	$1.38 \cdot 10^{-2}$
1.03	$8.51 \cdot 10^{-2}$	$2.34 \cdot 10^{-2}$	$4.78 \cdot 10^{-3}$
0.51	$1.86 \cdot 10^{-2}$	$5.14 \cdot 10^{-3}$	$9.41 \cdot 10^{-4}$
0.26	$3.23 \cdot 10^{-2}$	$1.48 \cdot 10^{-3}$	$2.52 \cdot 10^{-4}$

REVOLUTION OF A SPHERE AROUND THE DIAGONAL OF A DOMAIN



INITIAL



**MPDATA GAGE AFTER 1
REVOLUTION**

$$\frac{\partial \Phi}{\partial t} + \nabla \cdot (\mathbf{V}\Phi) = \mathbf{R}$$

NFT MPDATA: a general template

$$\Phi_i^{n+1} = \Phi_i^* + 0.5\delta t \mathbf{R}_i^{n+1}$$

$$\Phi^* \equiv \mathcal{A}(\Phi^n + 0.5\delta t \mathbf{R}^n, \widehat{\mathbf{V}}^{n+1/2})$$

$$R^{n+1} = R(t + \delta t) + \mathcal{O}(\delta t^3)$$

implicit integration

*preconditioned non-symmetric
Krylov-subspace elliptic solver*

explicit integration

$$\forall_i \quad \Phi_i^{n+1, \mu} = \Phi_i^* + 0.5\delta t \mathbf{R}_i^{n+1, \mu-1} \quad \mu = 1, \dots, m$$

Explicit integration

Compressible flows

(Smolarkiewicz, Szmelter JCP 2008 published on line)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{V} \rho) = 0$$

$$\frac{\partial q^I}{\partial t} + \nabla \cdot (\mathbf{V} q^I) = -\frac{\partial p}{\partial x^I} .$$

$$\frac{\partial e}{\partial t} + \nabla \cdot (\mathbf{V} e) = -p \nabla \cdot \mathbf{V}$$

Internal Energy Equation

$$\frac{\partial \Theta}{\partial t} + \nabla \cdot (\mathbf{V} \Theta) = 0$$

Potential Temperature Equation

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{V} E) = -\nabla \cdot (\mathbf{V} p)$$

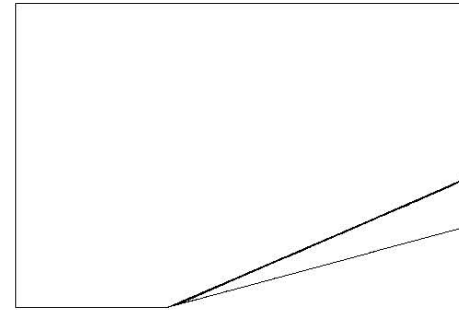
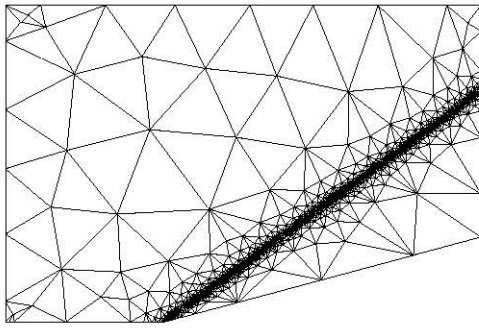
Classical Total Energy Equation

$$\frac{\partial E}{\partial t} + \nabla \cdot (\tilde{\mathbf{V}} E) = 0 \quad \tilde{\mathbf{V}} \equiv \mathbf{V}(1 + p/E)$$

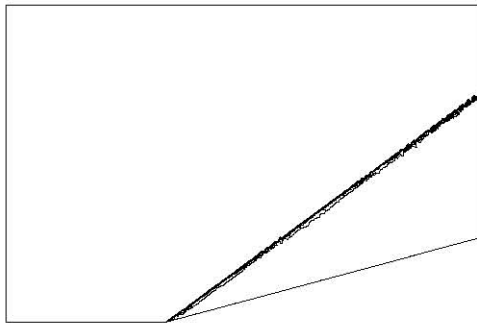
Modified Total Energy Equation

Supersonic flows

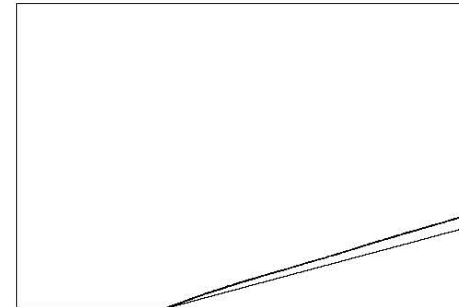
Mesh adaptivity by remeshing



$M = 5$



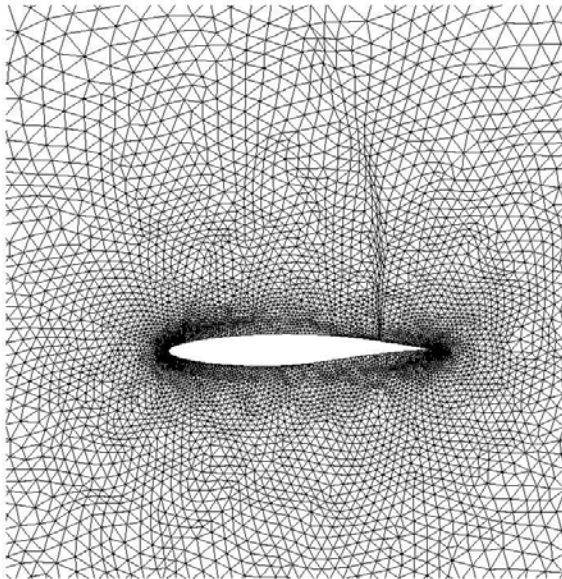
$M = 2.5$



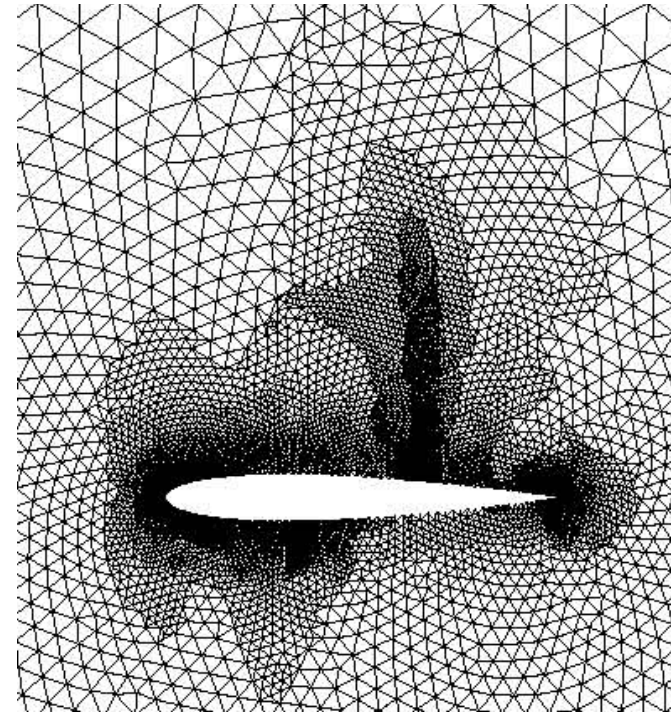
$M = 15$

ADAPTIVITY with a refinement indicator based on MPDATA lead error

(Szmelter, Smolarkiewicz IJNMF 2005)



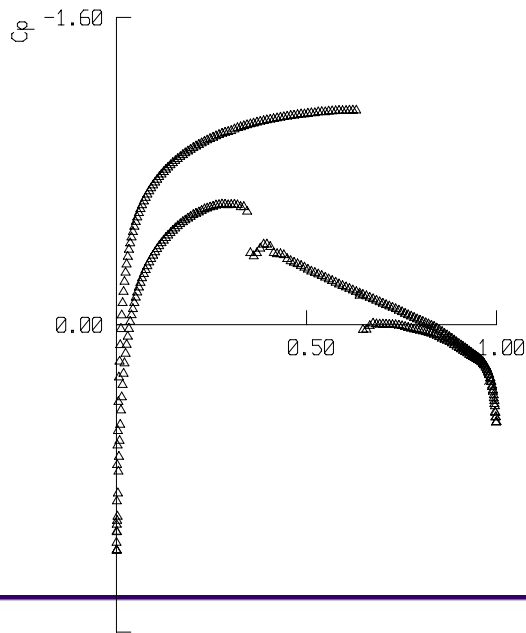
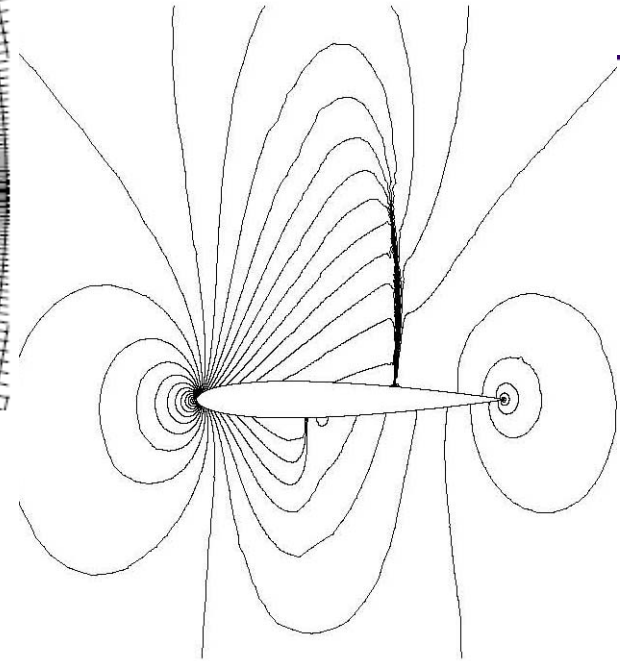
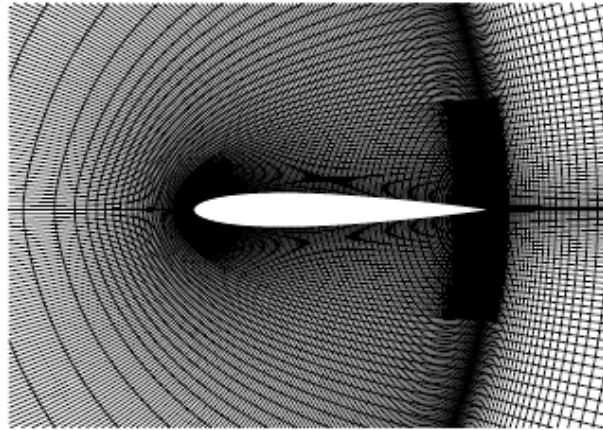
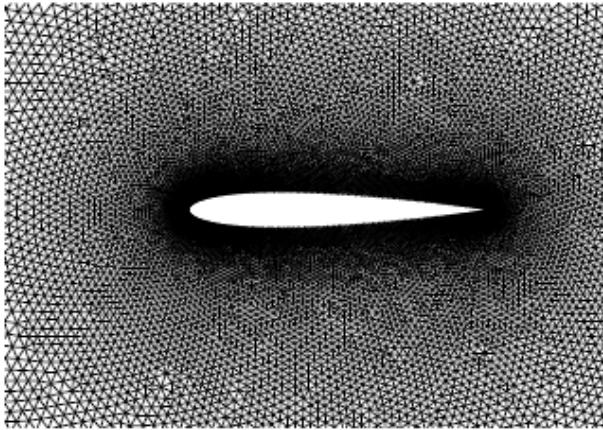
Mesh movement



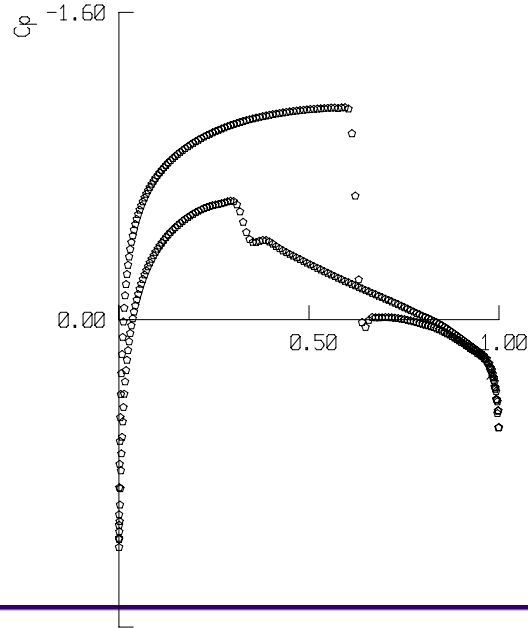
Point enrichment

Transonic flow

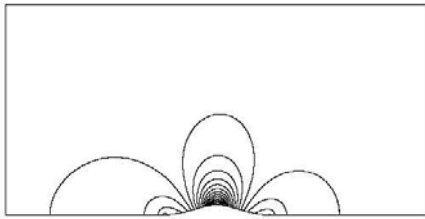
NACA012 $M=0.85$ $\alpha=1.25^\circ$



MPDATA



Runge-Kutta



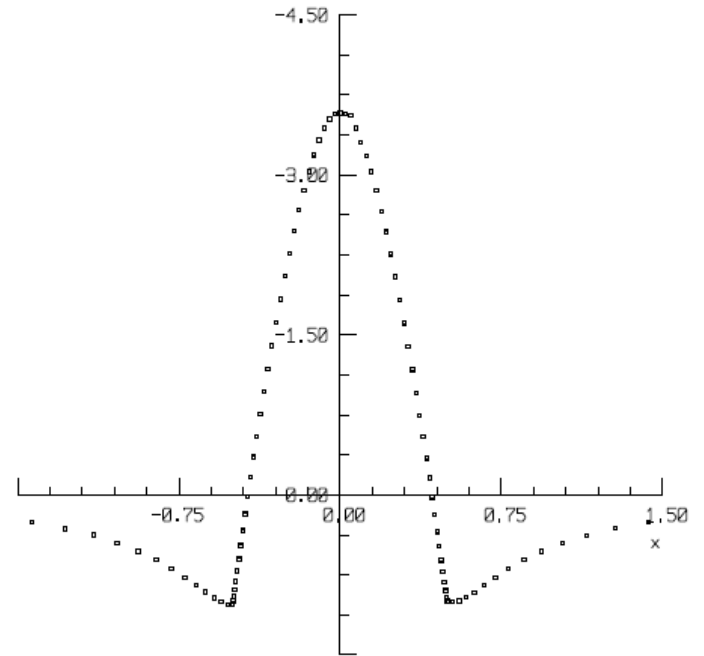
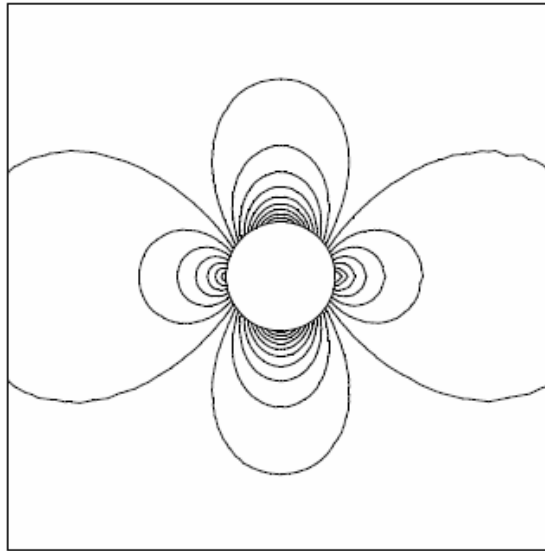
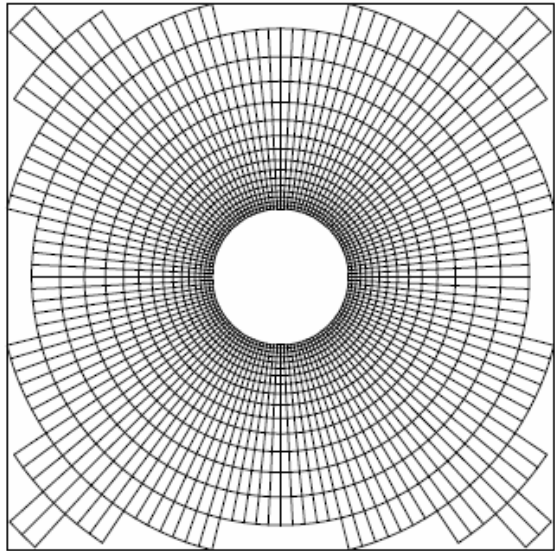
CONVERGENCE STUDY

MPDATA - NFT EULER SOLVER

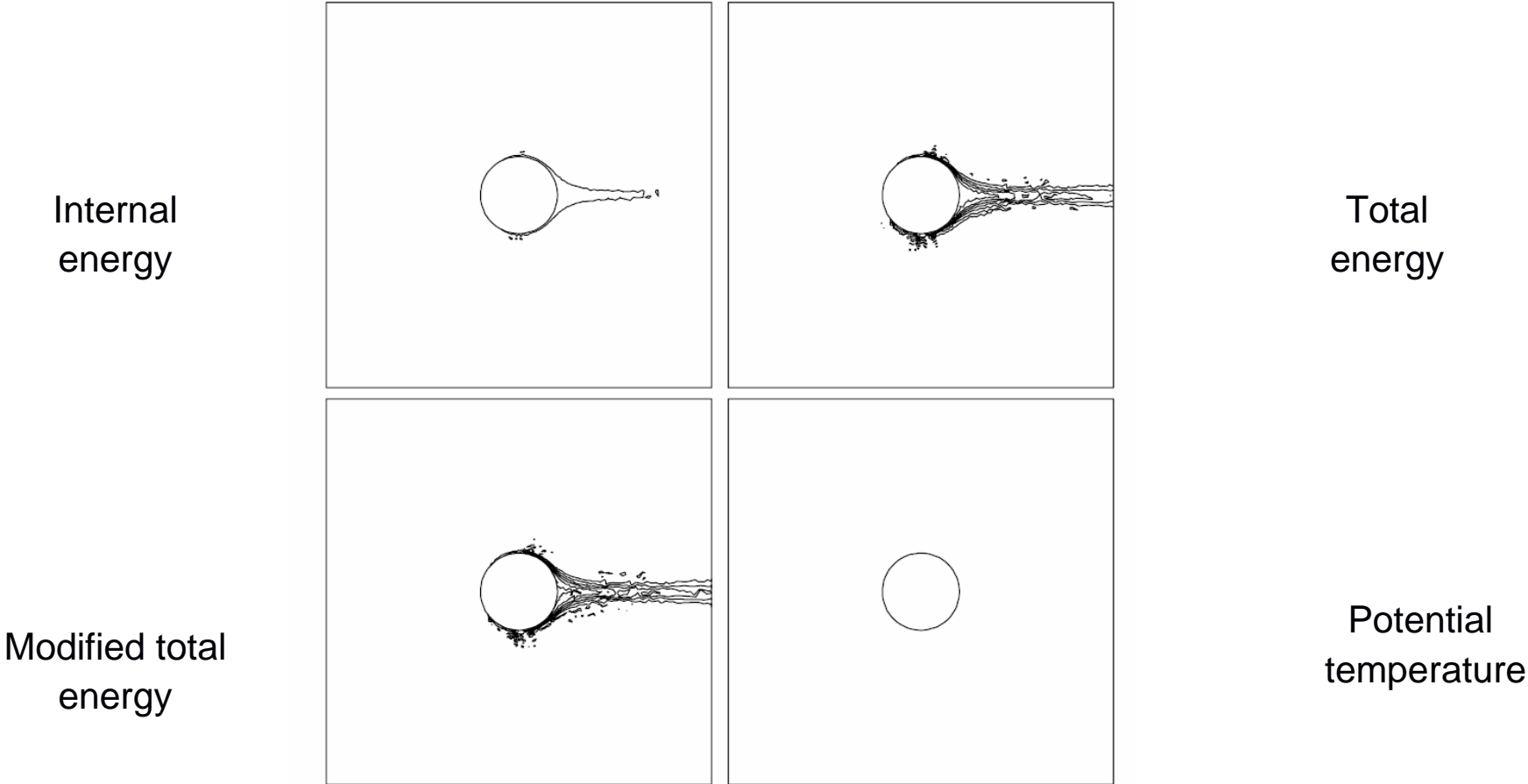
M=0.5

δ_E	MPDATA	L_2	UPWIND	L_1
$4.47 \cdot 10^{-2}$	$4.87 \cdot 10^{-3}$	$(5.47 \cdot 10^{-3})$	$1.48 \cdot 10^{-3}$	$(1.97 \cdot 10^{-3})$
$3.10 \cdot 10^{-2}$	$3.58 \cdot 10^{-3}$	$(4.18 \cdot 10^{-3})$	$1.19 \cdot 10^{-3}$	$(1.73 \cdot 10^{-3})$
$2.19 \cdot 10^{-2}$	$1.64 \cdot 10^{-3}$	$(2.83 \cdot 10^{-3})$	$7.04 \cdot 10^{-4}$	$(1.51 \cdot 10^{-3})$
$1.54 \cdot 10^{-2}$	$1.01 \cdot 10^{-3}$	$(2.17 \cdot 10^{-3})$	$4.36 \cdot 10^{-4}$	$(1.21 \cdot 10^{-3})$
$1.07 \cdot 10^{-2}$	$6.24 \cdot 10^{-4}$	$(1.58 \cdot 10^{-3})$	$2.38 \cdot 10^{-4}$	$(9.01 \cdot 10^{-4})$
$7.62 \cdot 10^{-3}$	$3.38 \cdot 10^{-4}$	$(1.19 \cdot 10^{-3})$	$1.25 \cdot 10^{-4}$	$(6.90 \cdot 10^{-4})$
$5.35 \cdot 10^{-3}$	$1.77 \cdot 10^{-4}$	$(8.57 \cdot 10^{-4})$	$6.61 \cdot 10^{-5}$	$(5.10 \cdot 10^{-4})$
$3.78 \cdot 10^{-3}$	$8.50 \cdot 10^{-5}$	$(6.06 \cdot 10^{-4})$	$2.92 \cdot 10^{-5}$	$(3.65 \cdot 10^{-4})$
$2.67 \cdot 10^{-3}$	$4.66 \cdot 10^{-5}$	$(4.34 \cdot 10^{-4})$	$1.79 \cdot 10^{-5}$	$(2.64 \cdot 10^{-4})$

Flow past a cylinder $M=0.38$



Flow past a cylinder $M=0.38$ --- Entropy deviation triangular meshes



Flow past a cylinder

Equations; MPDATA	Mach (Min,Max)	Pressure (Min,Max)	Σ (Min,Max)
<u>Structured 128×33 O-grid</u>			
internal energy (16)	0.00000,0.91	0.64,1.11	-0.00002,0.00021
total energy (17)	0.00000,0.91	0.62,1.11	-0.00005,0.00081
total energy (18)	0.00000,0.91	0.63,1.11	-0.00022,0.00125
potential temp. (19)	0.00000,0.91	0.62,1.11	-0.00000,0.00001
<u>Unstructured triangular mesh</u>			
internal energy (16)	0.00001,0.90	0.64,1.11	-0.00037,0.00053
total energy (17)	0.00000,0.90	0.63,1.11	-0.00098,0.00247
total energy (18)	0.00000,0.90	0.63,1.11	-0.00130,0.00406
potential temp. (19)	0.00000,0.90	0.62,1.11	-0.00005,0.00005
Scheme; after [52]	Mach (Min,Max)	Pressure (Min,Max)	Σ (Min,Max)
MUSCL	0.0001 ,0.82	0.67,1.10	-0.0004 ,0.048
Abgrall's blended	0.0001 ,0.89	0.64,1.11	0.0 ,0.009
LDA	0.0 ,0.94	0.62,1.10	-0.001 ,0.010

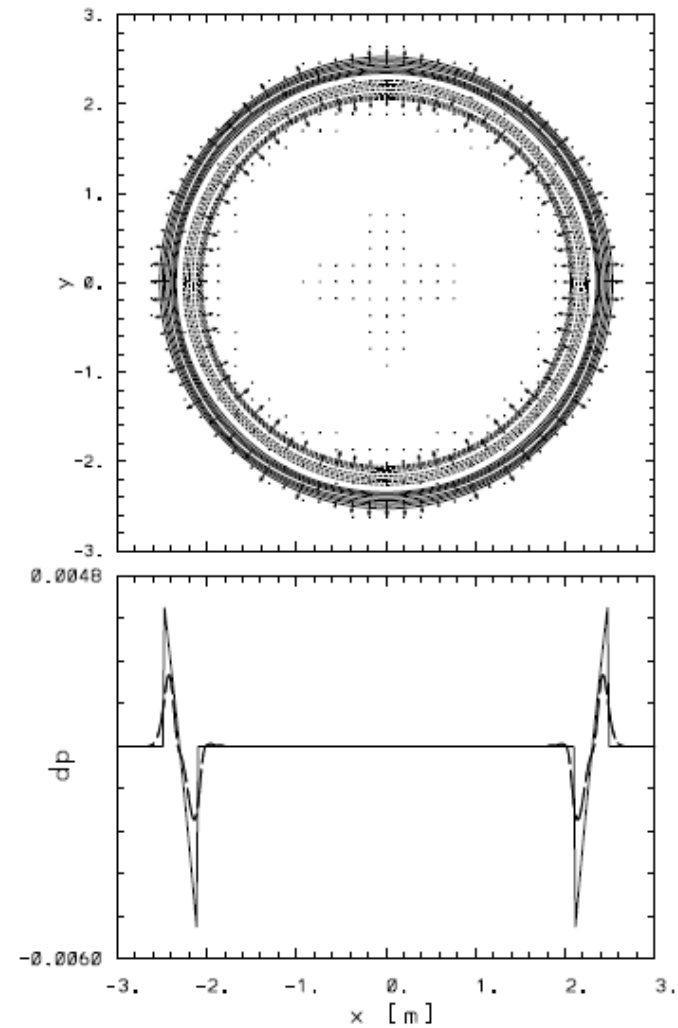
$$M=0$$

$$\delta p = (p - p_o)/p_o \text{ at } y = z = 0$$

$$t \gg r_o/c_o$$

3D Spherical wave; Analytical solution

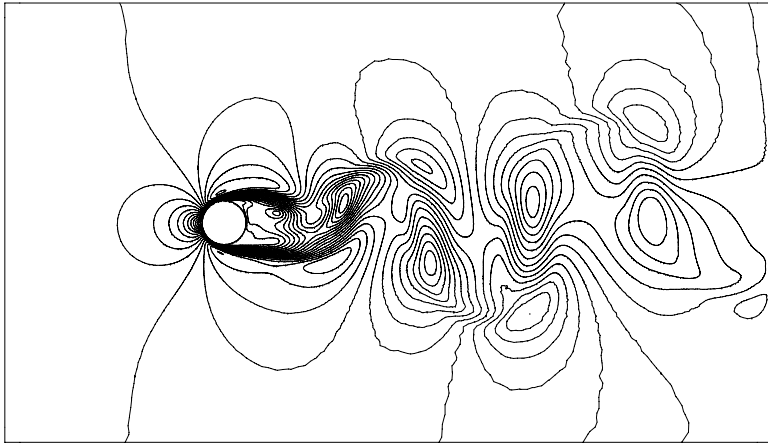
--- Landau & Lifshitz



Implicit integration

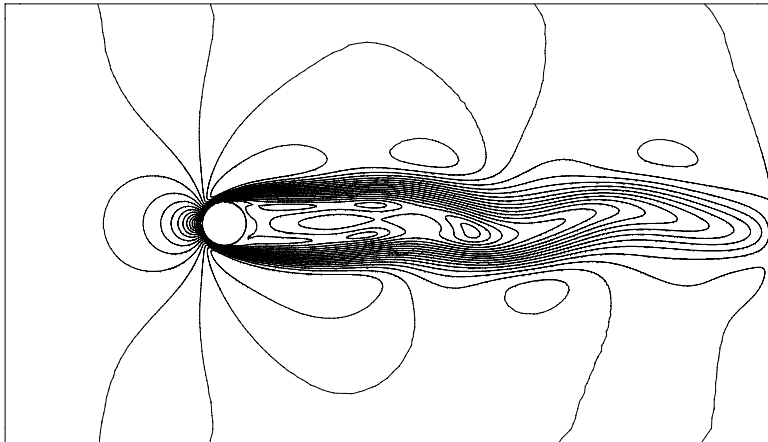
Incompressible flows

Incompressible flows



$Re=200.$

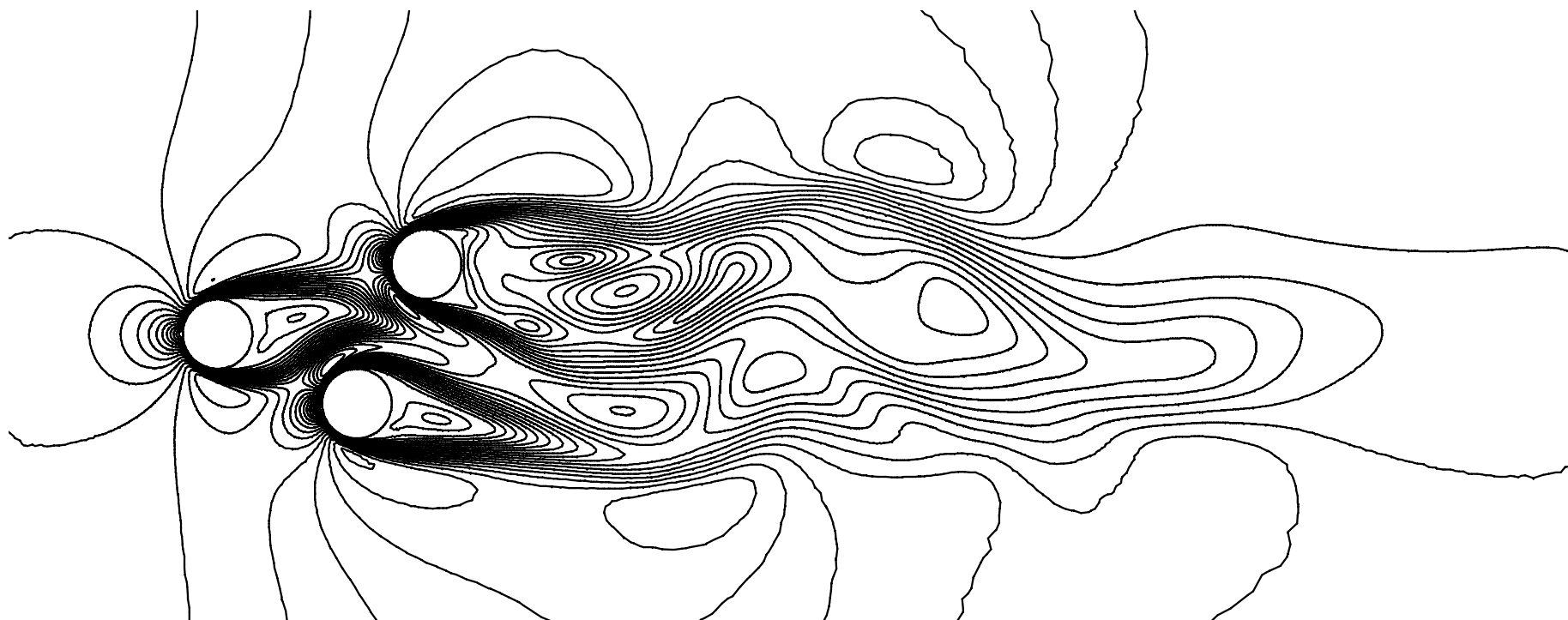
Strouhal number = 183



$Re=100.$

Strouhal number = 163

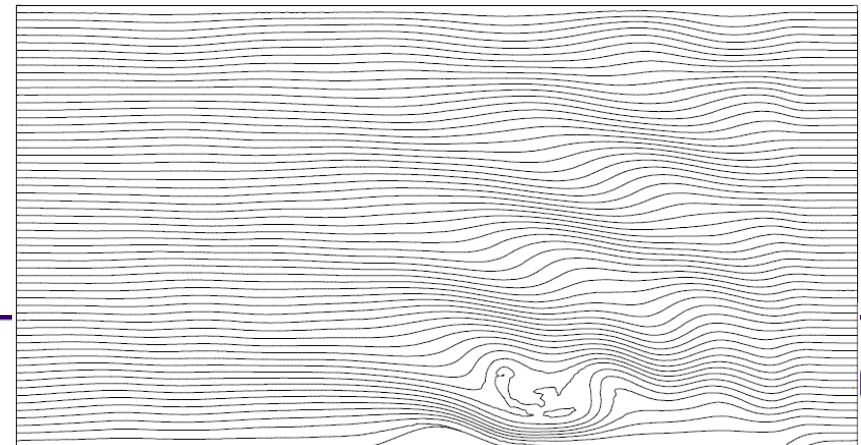
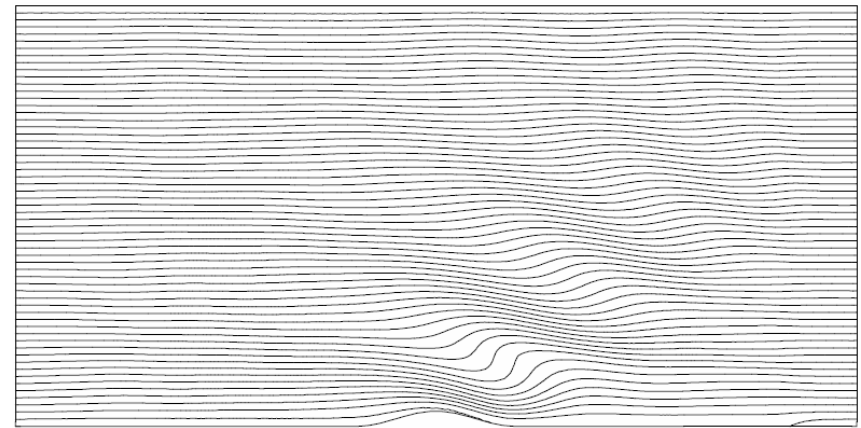
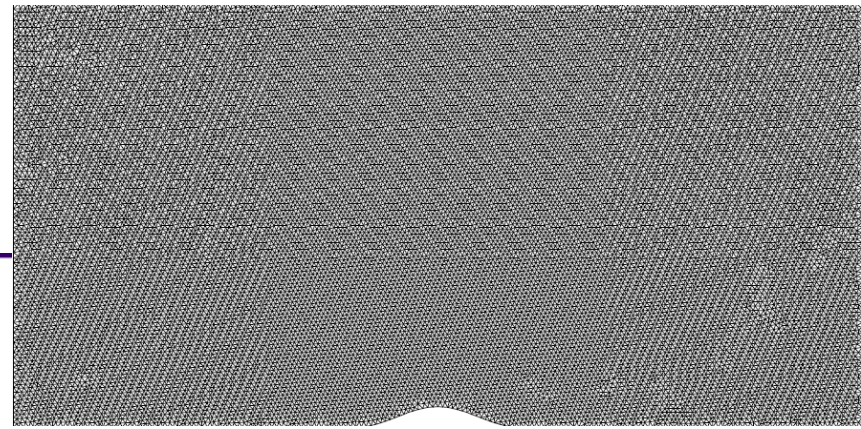
Incompressible flows --- multi-connected domains



Re=100

*2D – non-hydrostatic model
Incompressible Boussinesq
ILES*

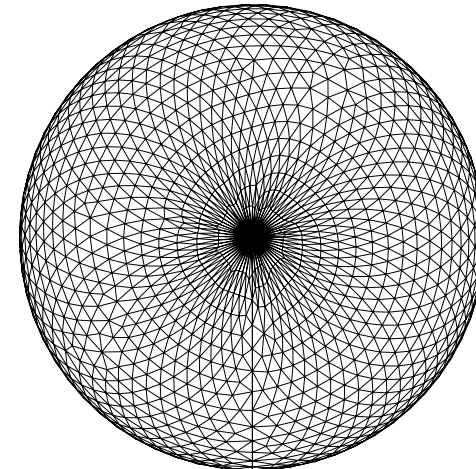
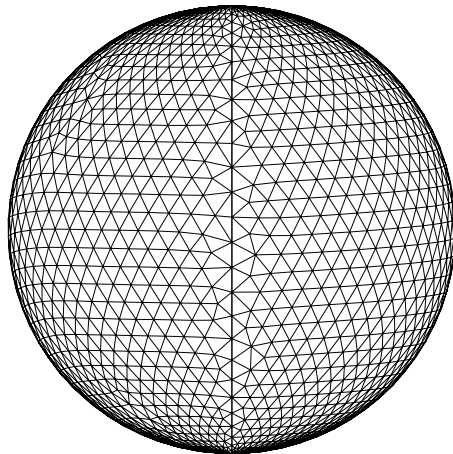
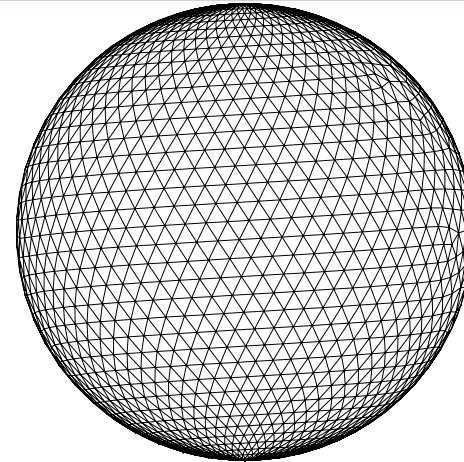
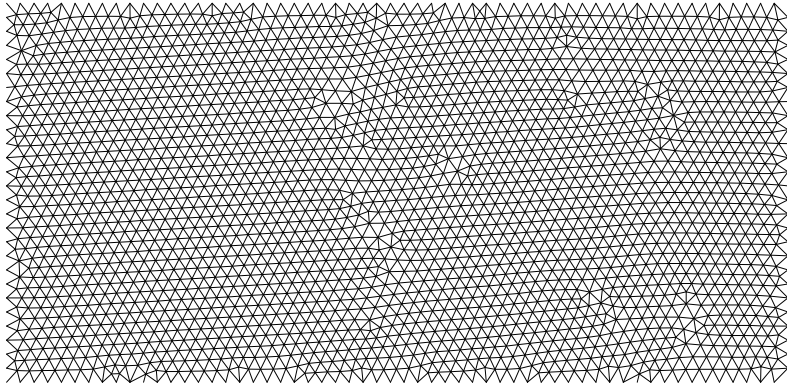
*Orographically forced
atmospheric gravity waves*



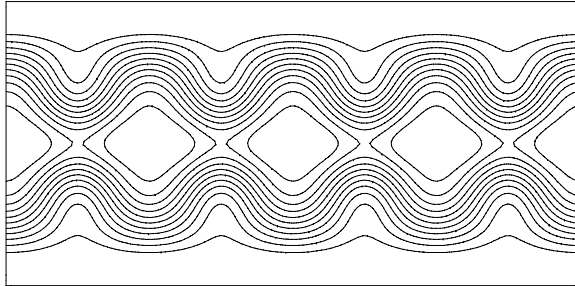
*$Fr < Fr_{critical}$
vertical wave propagation*

*$Fr > Fr_{critical}$
wave breaking*

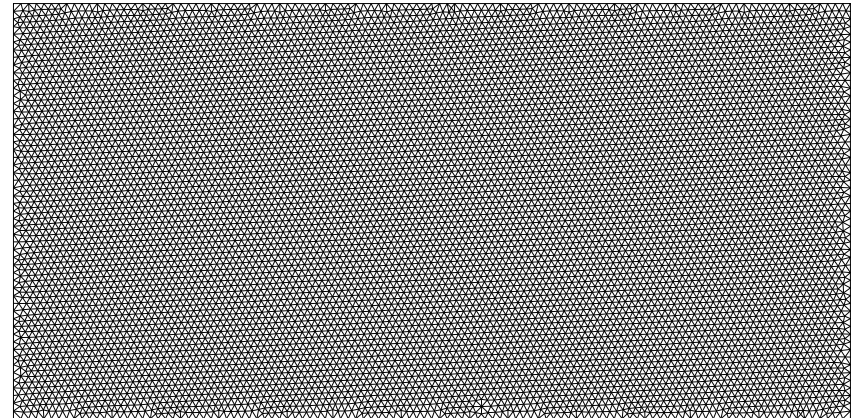
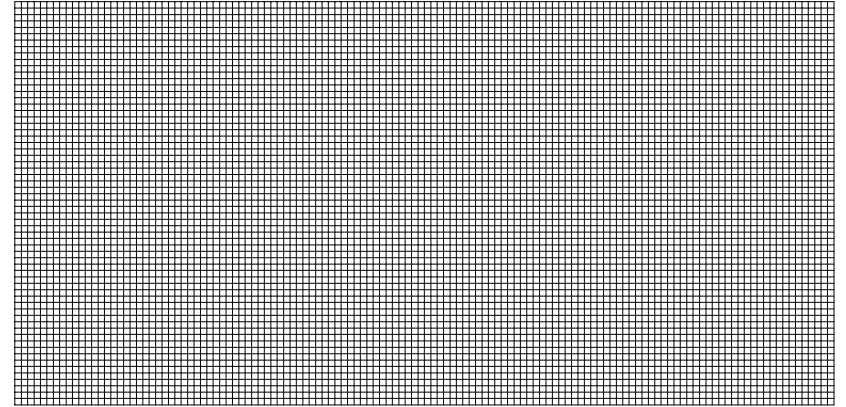
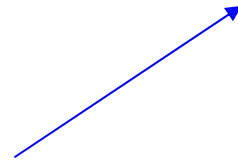
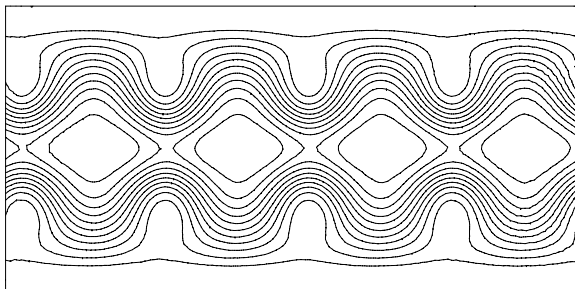
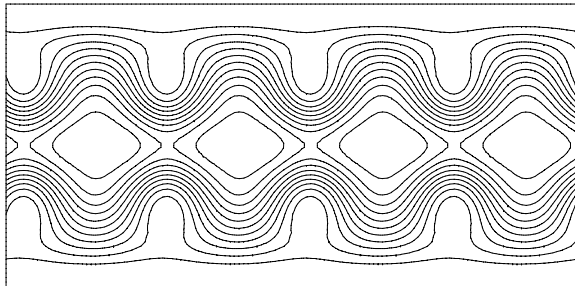
Flows on a Sphere --- Geospherical coordinates



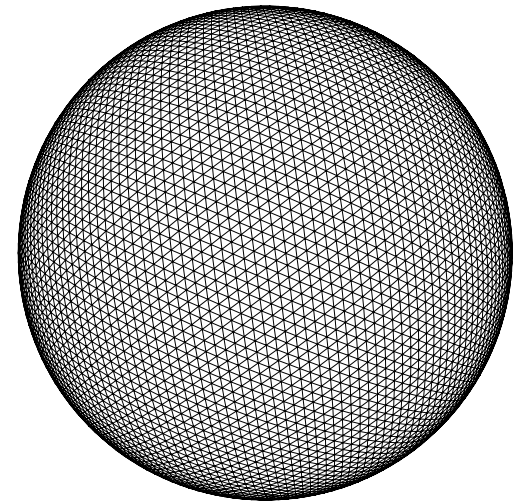
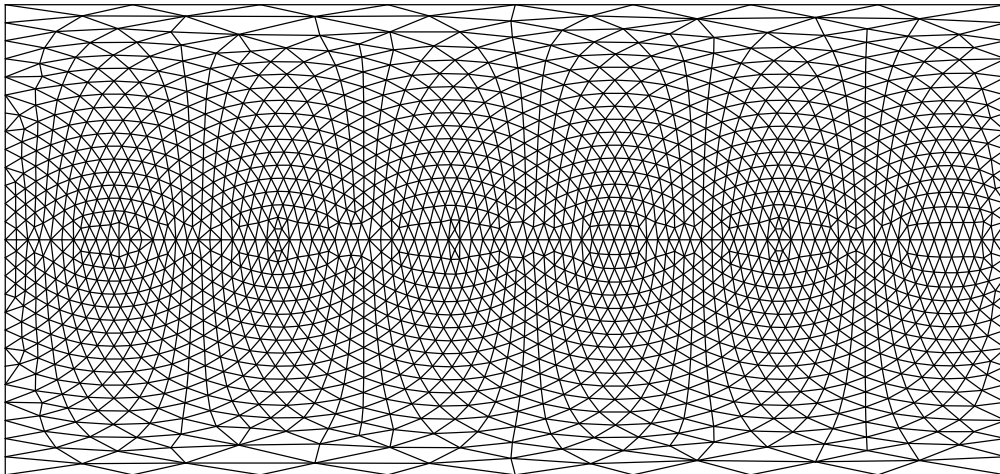
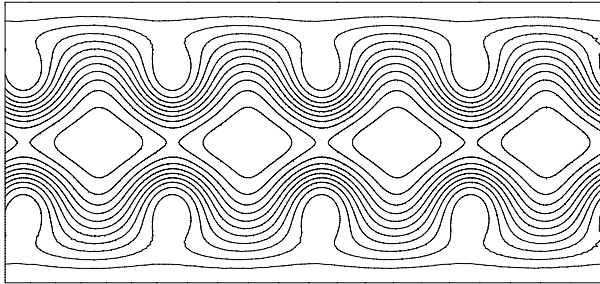
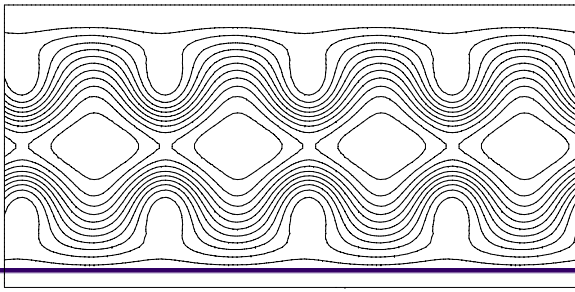
Shallow water equations



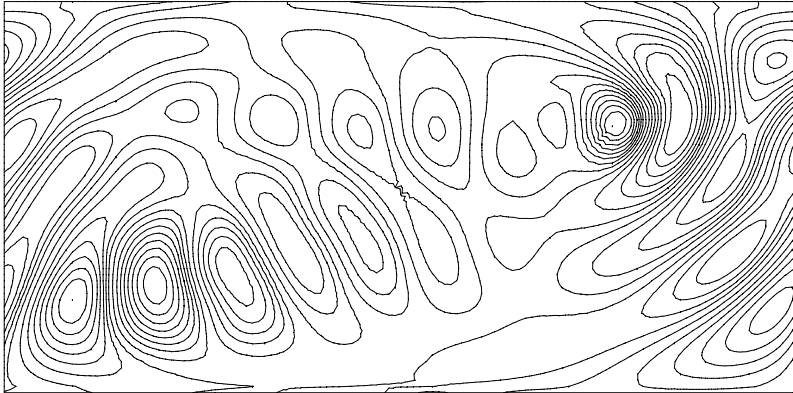
initial



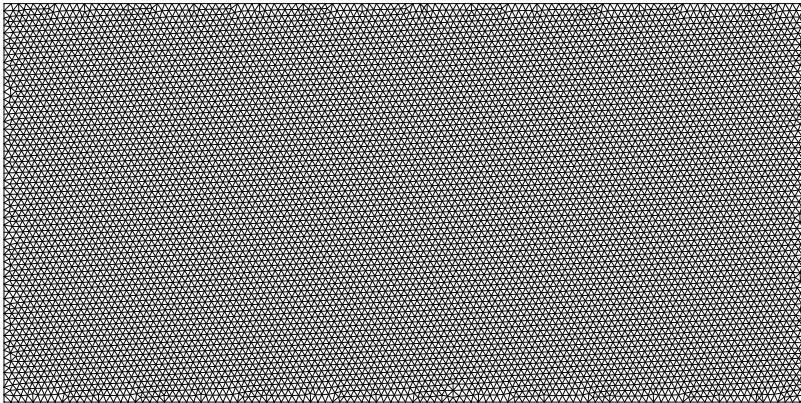
Shallow water equations



Shallow water equations

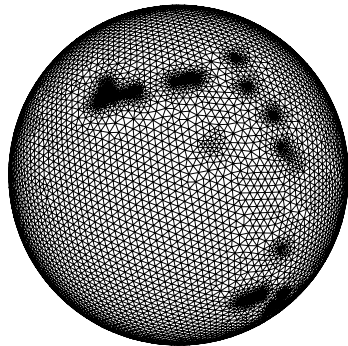
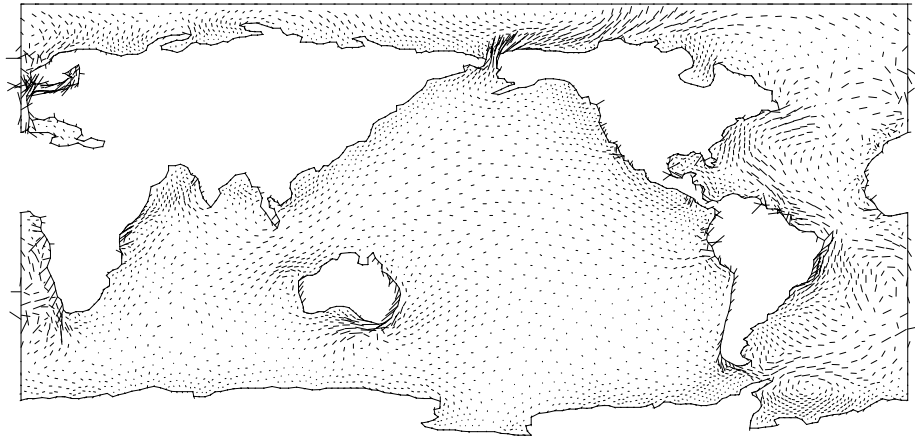
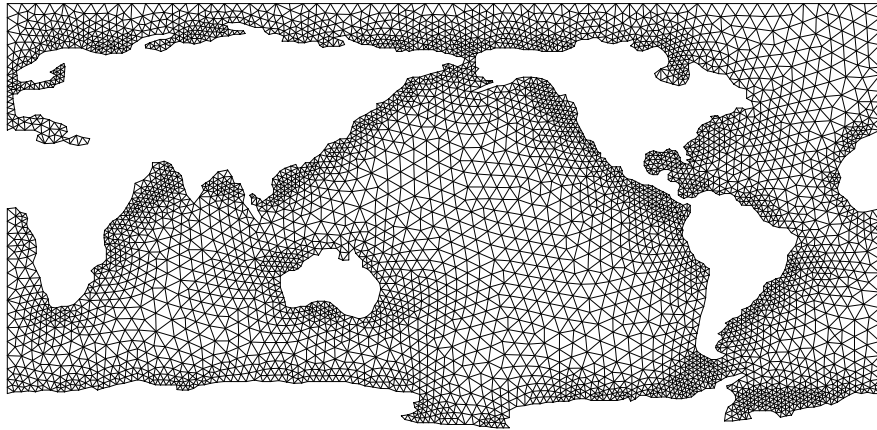


Zonal flow over a cone



Potential for modelling of multi-connected domains
and easy implementation of mesh adaptivity.

(David Parkinson)



*(Treatment of hanging nodes & hybrid meshes
Szmelter et al Comp. Meth. Appl. Mech. Eng 92)*

CONCLUSIONS

- Presented work opens avenues to construct a flexible edge-based clone of EULAG and to study unstructured meshes performance for all-scale atmospheric flows.
- Main new effort lies in mesh generation, visualisation and parallelisation.