解適合格子法による流体解析の高解像度化
High Resolution Fluid Simulation by Adaptive Mesh Refinement

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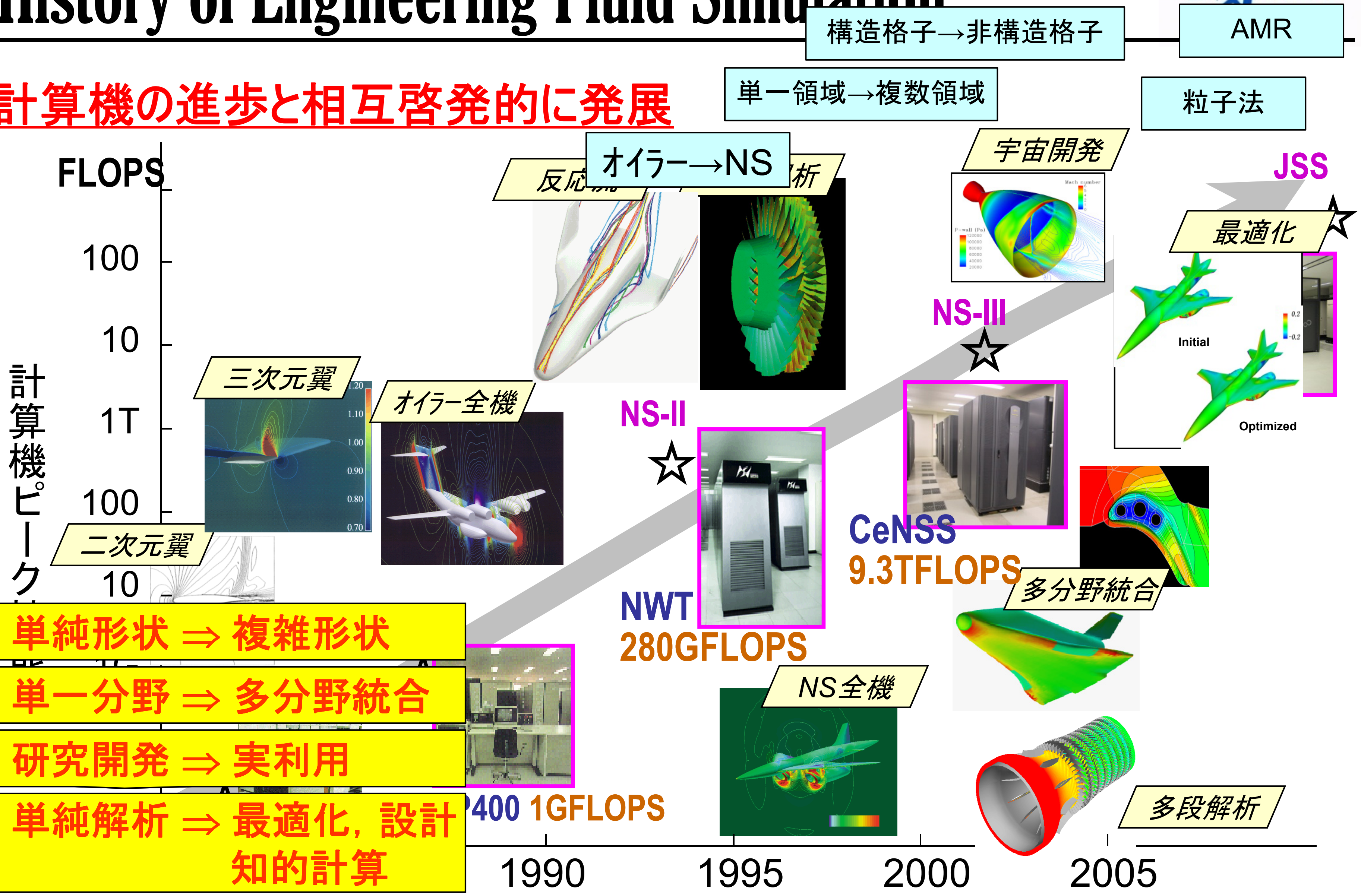
2011.12.9

TOC

- Recent trend of engineering fluid simulation
- Research background
- AMR methodology used
  - Structured, Octree-based, Parallelization with load balance
- Computational results and discussion
- Summary

History of Engineering Fluid Simulation

計算機の進歩と相互啓発的に発展



単純形状 ⇒ 複雑形状

単一分野 ⇒ 多分野統合

研究開発 ⇒ 実利用

単純解析 ⇒ 最適化，設計
知的計算

JAXA流体解析の最近の状況

- 工学
  - より現実的（複雑）な状況の取り扱い
    - 複雑形状，非定常，構造変形，反応・混相
  - 設計や開発との連携，課題解決
    - 空力音響，空力加熱，設計探査・パラスタ，制御・最適化
  - 可能性提示から実開発利用へ

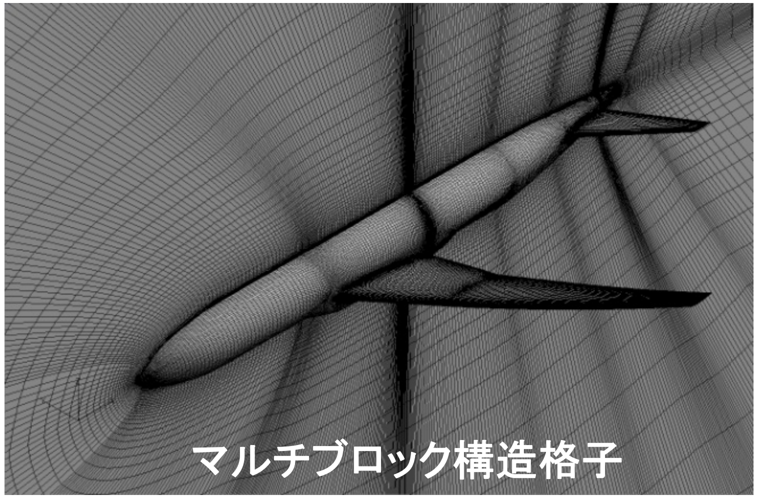
- 学術
  - 乱流・遷移，不安定・混合
    - 複雑乱流（剥離流，噴流），大規模化は停留（N~Re^9/4）
  - 燃焼，プラズマ
    - 予混合/拡散/超音速，火炎，噴霧・液滴，粒子系

技術トピックス・課題

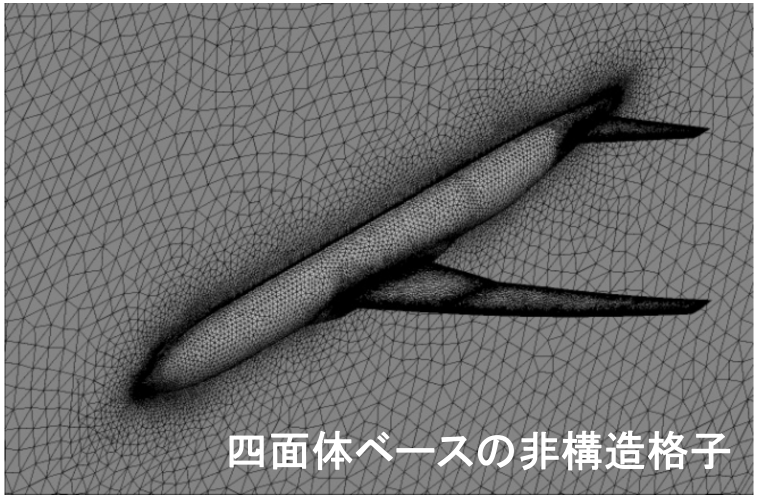
- 格子
  - 構造/非構造/ハイブリッド/グリッドレス，人手/自動
  - マルチブロック/オーバーセット/解適合
- 解法
  - 非定常・時間依存計算（DNS/LES/DES）
    - DNS: Direct Numerical Simulation
    - LES: Large-Eddy Simulation
    - DES: Detached Eddy Simulation
  - 高次精度（WENO，COMPACT，DG）
  - カーバンクル，熱流束予測，壁面モデル，高速化
- 可視化，その他
  - 並列化，スケール性，大規模データ処理，データ同化

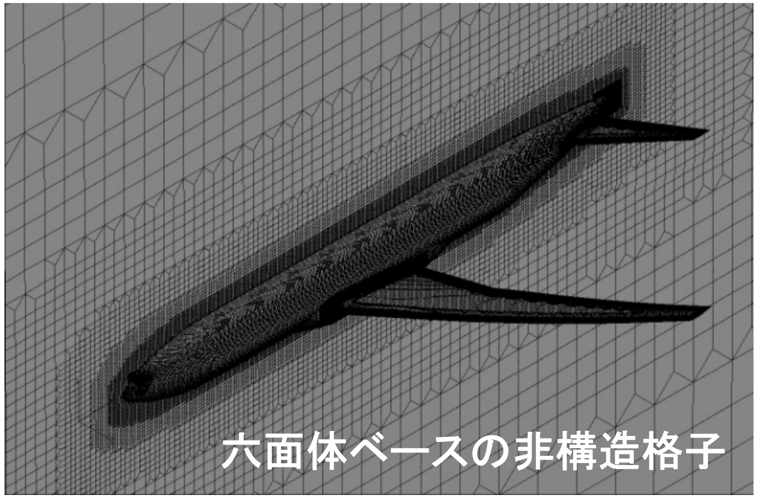
実用解析における格子

- 構造格子: 格子点が規則的に配置されている格子



- 非構造格子: 格子点が不規則に配置されている格子

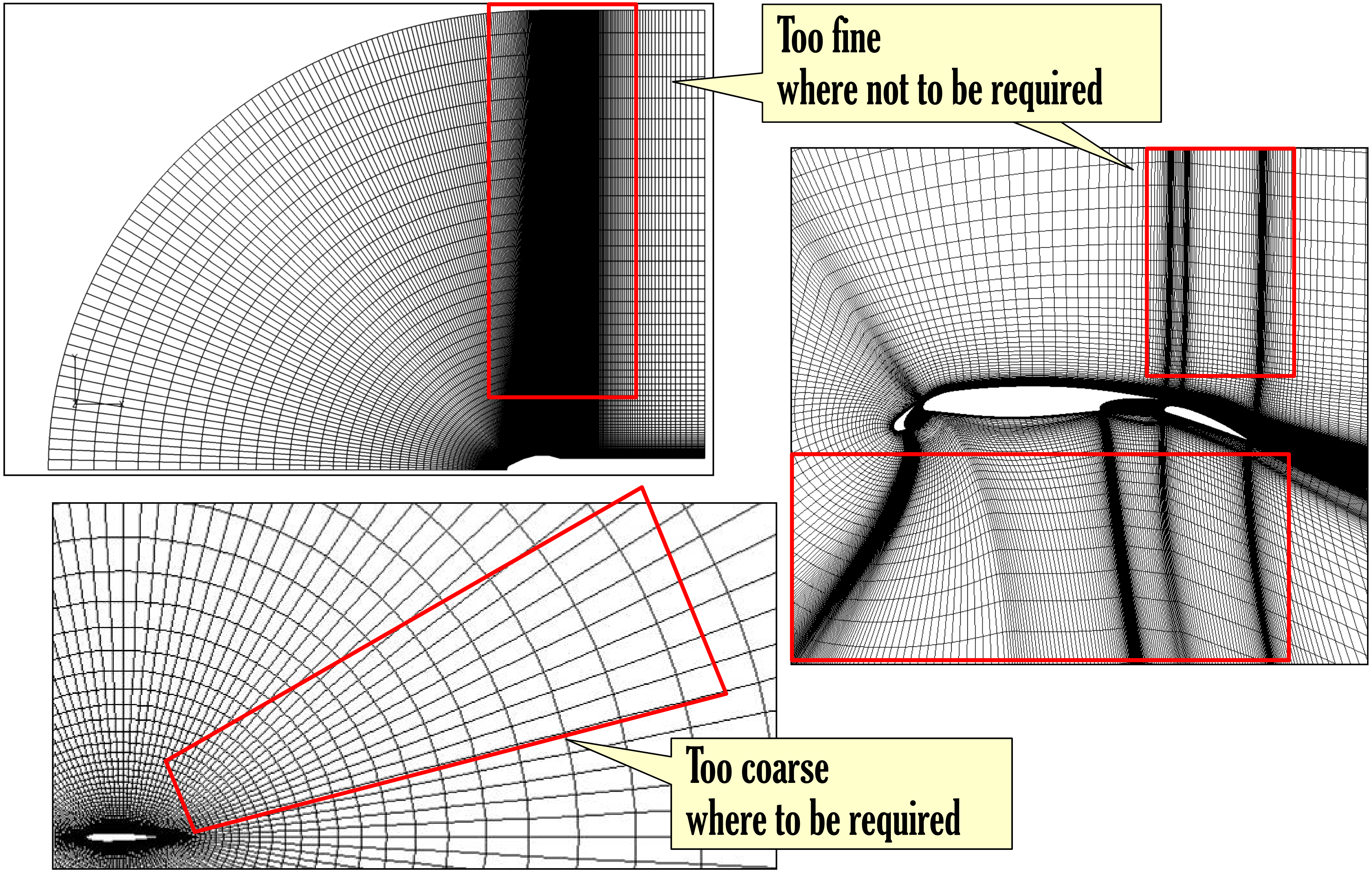




Research Background

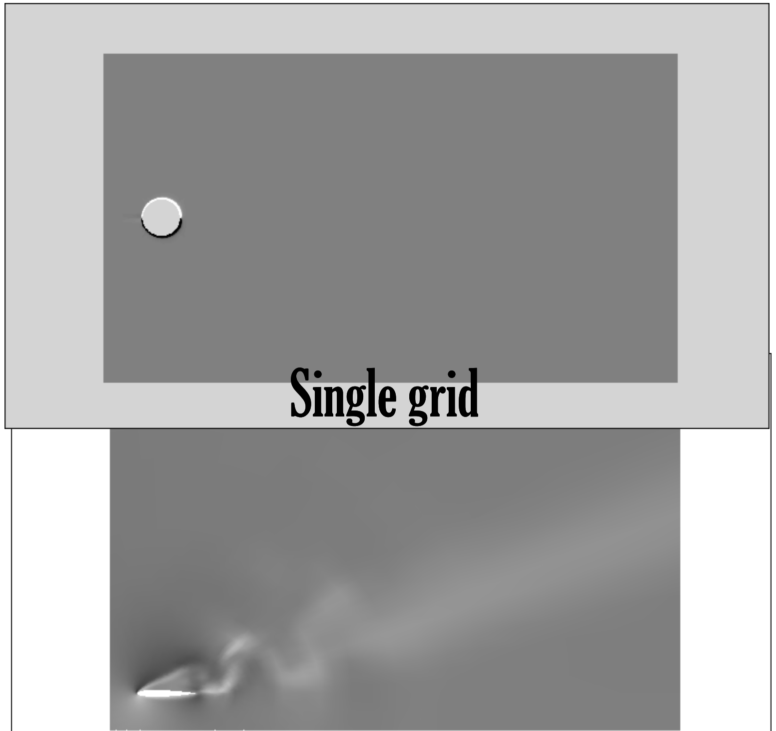
- In the researches on practical aerodynamic problems i.e. aeroacoustics, flow control, fluid-structure interaction as flutter, the need for high-accuracy time-dependent unsteady flow simulation is being increased.
- For the unsteady flow simulations, DNS/LES/DES methods are becoming popular these days.
- On these methods, structured grid approach is still mainly used because high accuracy schemes like WENO, compact can be easily applied.
  - Unstructured, although suited for complicated geometry, is at most 2nd order.
- However, the proper mesh distribution for a structured grid is difficult to realize in actual cases, particularly in 3D, memory and CPU time limit is unavoidable.

Structured Mesh for DNS/LES/DES

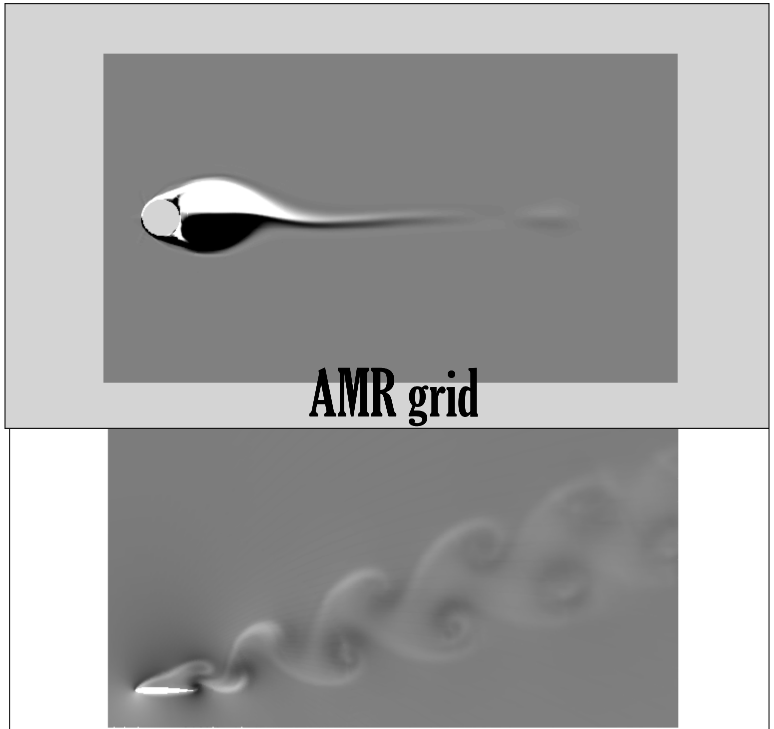


AMR Concept

- AMR: Adaptive Mesh Refinement is promising, effective
  - Practical flow phenomena is of multi-scale in terms of space and time
  - Area of required high resolution is limited
  - But, uniformly fine mesh leads to the increase of memory usage and CPU time
  - Fine mesh should be used only to where a high resolution is required



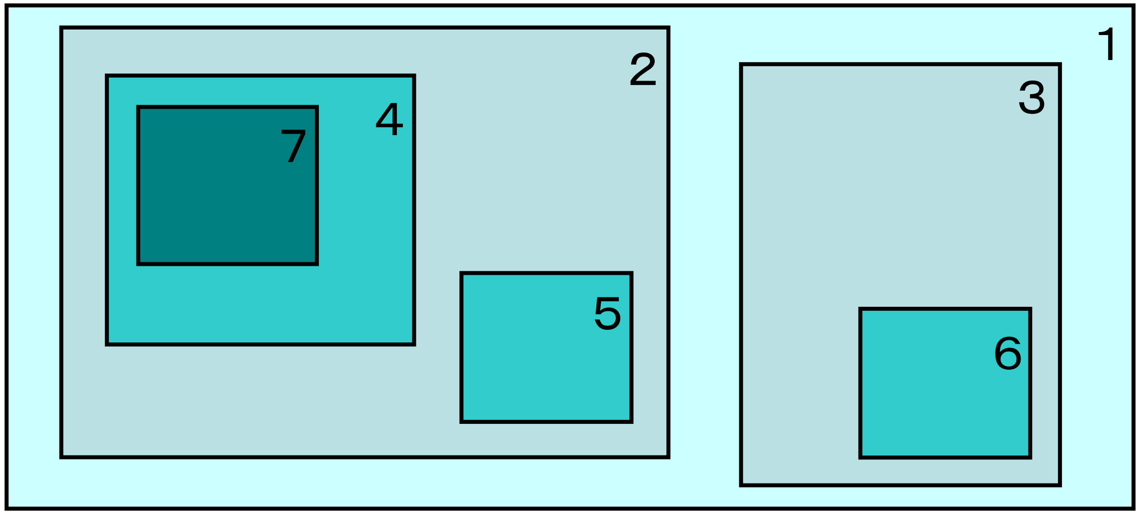
Single grid



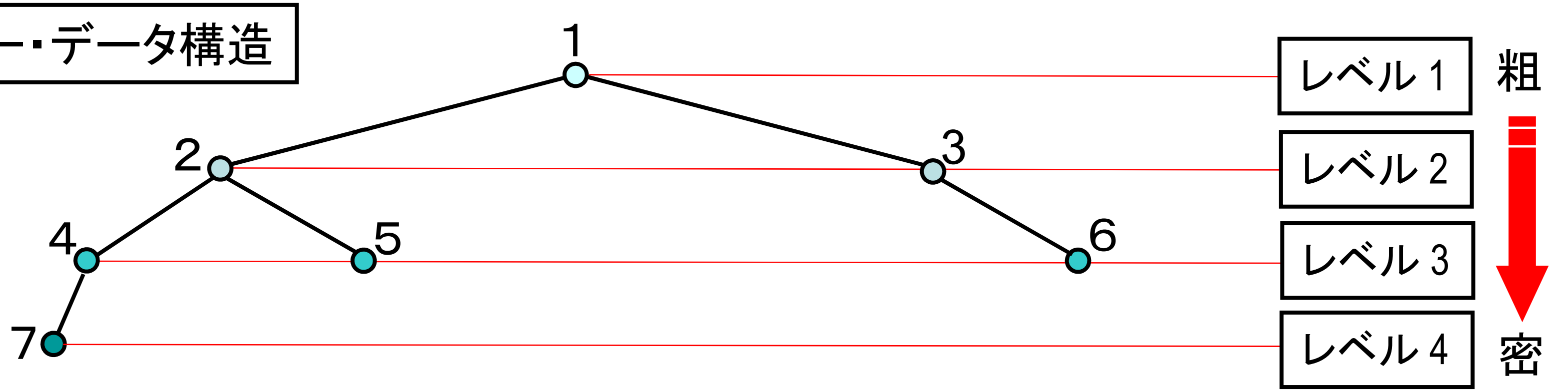
AMR grid

AMR Concept(2)

計算空間上のイメージ



ツリー・データ構造



Current Situation

- These days, there are many open AMR libraries freely available.
  - e.g. AMROC, Chombo, PARAMESH, SAMRAI, ENZO, Flash, RAMSES
- Our target is to apply AMR-based CFD to practical problems in aerospace engineering we are faced with at JAXA.
- Then, we have two choices;
  - to use the open AMR libraries and apply any one to our cases,
    - Object-oriented, Performance problem, Not easy to use
  - to develop our own AMR framework.
    - Flexible, Scalable, Practical, Work and time

AMR History

- 始まりは結構古い
  - M.J. Berger and J. Oliger, Adaptive Mesh Refinement for Hyperbolic Partial Differential Equations, JCP 53, 484-512, 1984
  - M.J. Berger and P. Colella, Local Adaptive Mesh Refinement for Shock Hydrodynamics, JCP 82, 64-84, 1989
  - M.J. Berger and R.J. LeVeque, An Adaptive Cartesian Mesh Algorithm for the Euler Equations in Arbitrary Geometries, AIAA 89-1930
- CG, Computer Science，代数幾何が起源？
- 米国で主に発展
  - ASCI計画（原爆のシミュレーション）と関係？

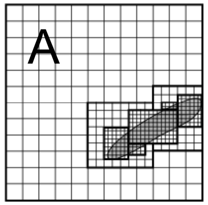
AMR History(2)

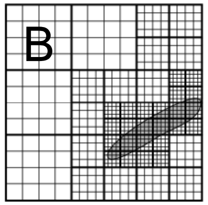
- 先駆的活動
  - Colella （LBNL） Chombo
    https://seesar.lbl.gov/ANAG/chombo/
  - MacNeice （Drexel U.） PARAMESH
    http://www.physics.drexel.edu/~olson/paramesh-doc/Users_manual/amr.html
  - Hornung （LLNL） SAMRAI
    https://computation.llnl.gov/casc/SAMRAI/SAMRAI_Applications.html
  - Aftosmith （NASA Ames） CART3D
    http://people.nas.nasa.gov/~aftosmis/cart3d/
- 日本では（航空宇宙では）あまりやられていない
  - 理由は不明，天文分野では盛ん

AMR Status

- 天文・宇宙論・MHD分野で盛ん

Code	Authors	Targets	Grid type	License	MHD
ORION	R. Klein	Star formation	A	Limited	Y
Enzo	M. Norman	Cosmology	A	Open	Y
FLASH	U. Chicago	Any	B	Open	Y
BATSRUS	K. Powell	Space weather	B	-	Y
NIRVANA	U. Ziegler	Any	B	Open	Y
RIEMANN	D. Balsara	ISM	A	Limited	Y
RAMSES	R. Teyssier	Cosmology	C	Open	Limited
ART	A. Kravtsov	Cosmology	C	Limited	N
AMRVAC	G. Toth	Any	A	Open	Y
SFUMATO	T. Matsumoto	Star formation	B	Limited	Y



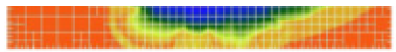


A:　パッチ式ブロック
B:　自己相似式ブロック
C:　セルベース

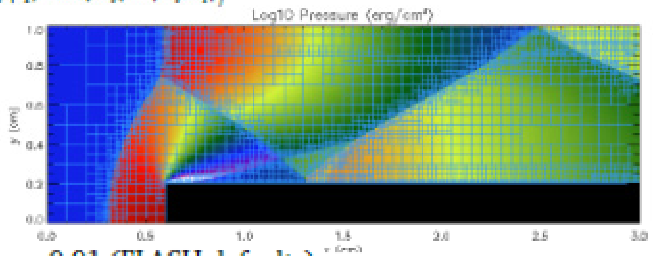
AMR Pros/Cons

- メリット
  - 少ない格子で高解像度，格子点の有効利用可能
  - 現象のスケール差が大きい場合に有効
  - 並列，MGと好相性
  - Shock capturing特性
  - MBより格子生成容易

Used to capture shocks. Compute scaled second derivative for each zone after Löhner (1987):



$$E_i \equiv \frac{|u_{i+1} - 2u_i + u_{i-1}|}{|u_{i+1} - u_i| + |u_i - u_{i-1}| + \epsilon\left(|u_{i+1}| + 2|u_i| + |u_{i-1}|\right)}$$



Refine block if

$$max_{block}\, E_i > C_1$$

Derefine block if

$$max_{block}\, E_i < C_2$$

Typical values $C_1 = 0.8$, $C_2 = 0.2$, $\epsilon = 0.01$ (FLASH defaults)

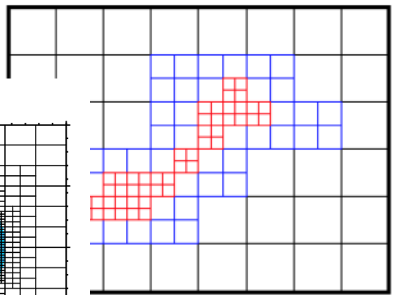
- デメリット
  - プログラミングの面倒，メモリ必要
  - 計算性能と相反

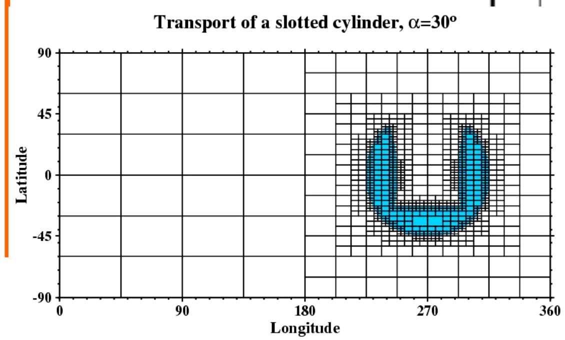
AMR特有の技術・課題

- 細分化方針，補間，ガードセル
- 並列化，オーダリング，探索
- 時間積分
- コーディング，データ構造
- 理論的課題
  - 解の一意性，収束性
- 技術的課題
  - 補間精度，保存性

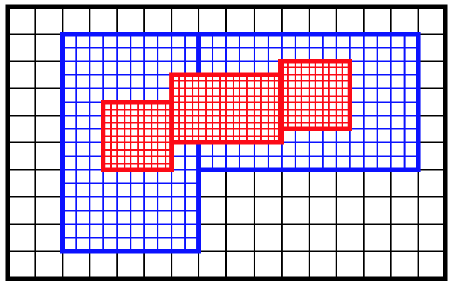
Cell-based vs Block-based

- Refine mesh cell-by-cell
  （Cell-based AMR）
- Flexible and efficient refinement patterns.
- Cut-cell is mainly used, but hard to deal with complex boundary shape.
- Large tree data structure to keep track of cells and their neighbors.
- Need to develop own flow solver, own pre-/post-software.

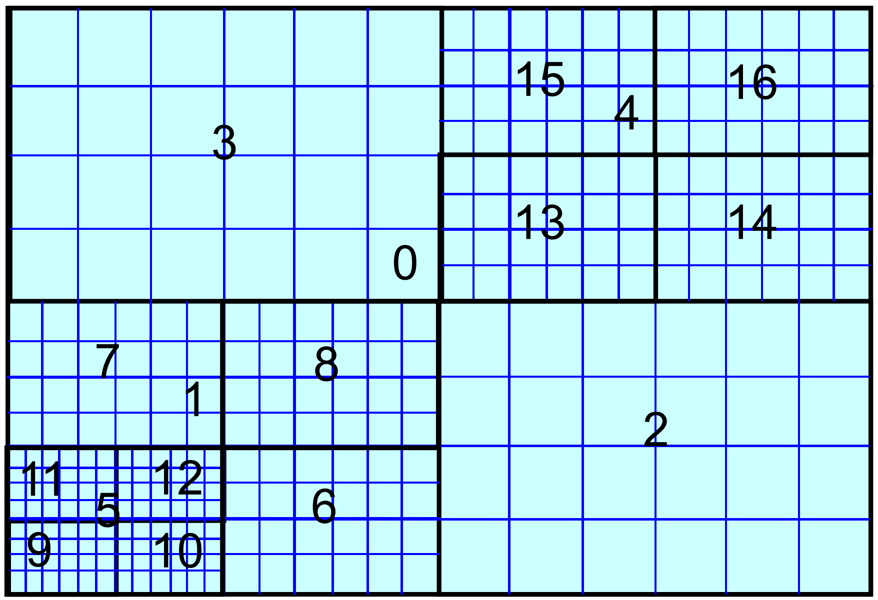




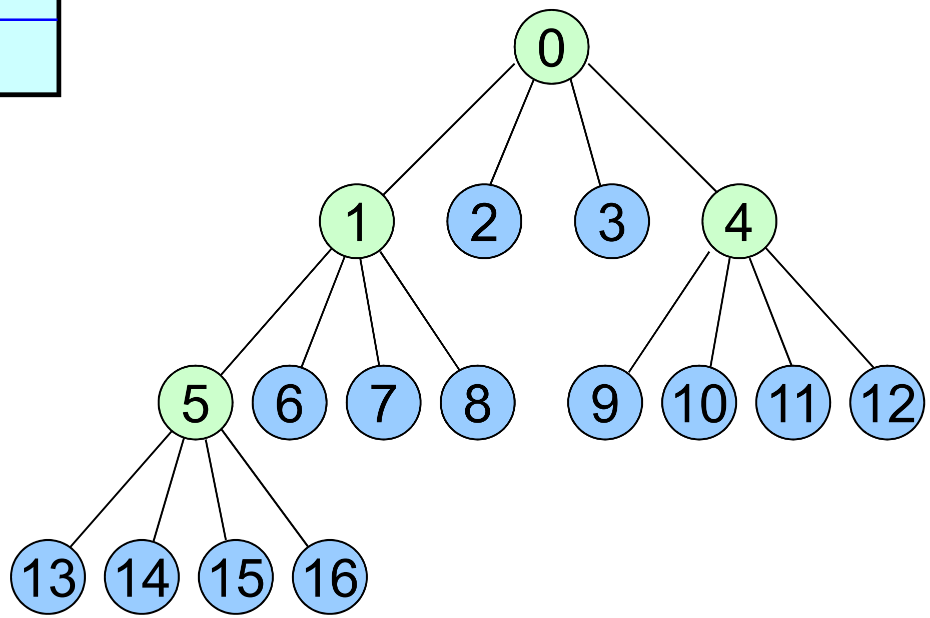
- Refine mesh block-by-block
  （Block-based AMR）
- May enable reuse of most of a legacy code designed for a structured mesh .
- Data communication only at block boundary.
- Easy data manipulation for statistical analysis in DNS/LES/DES.
- Hard to deal with complex boundary shape.



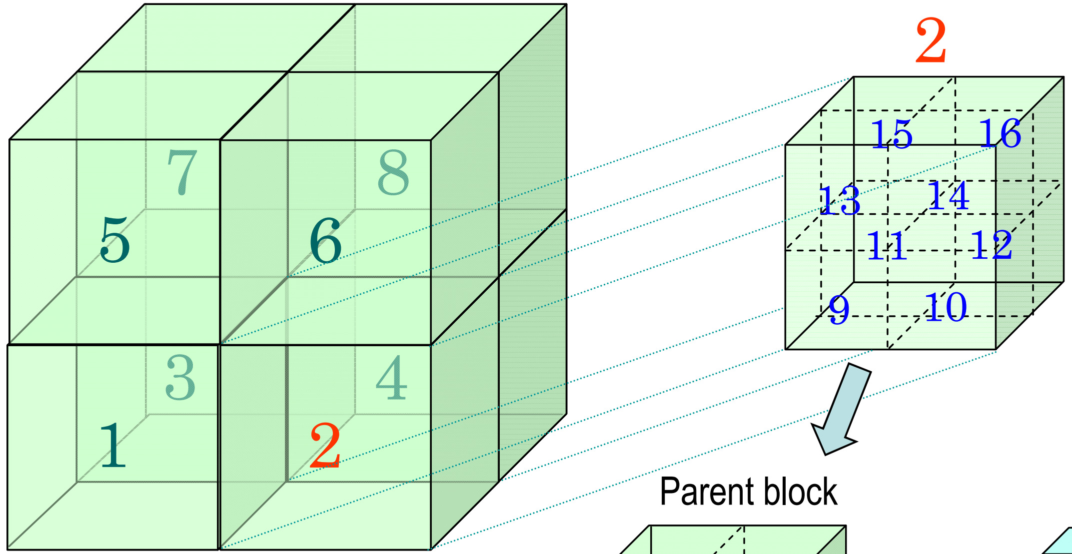
Data Structure by Self-Similar Tree



- A block is divided into Quadtree in 2D, Octree in 3D.
- Self-similarly organized tree
  ⇒ Each block has the same number of grid points.

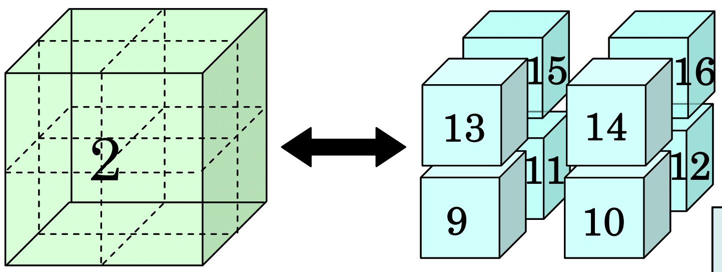


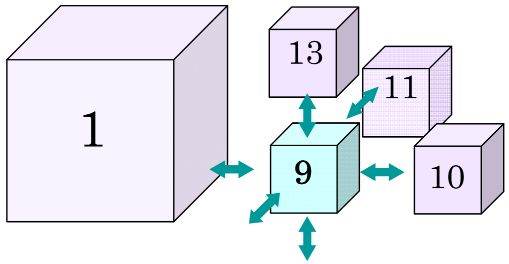
Managing Octree-Based Data Structure



Parent block

Child block





neigh(1, 9) = 1
neigh(2, 9) = 10
neigh(3, 9) = -20 → Physical Boundary
neigh(4, 9) = 11
neigh(5, 9) = -20 → Physical Boundary
neigh(6, 9) = 13

Face ID   Block ID

A work block with BlockID has,

- **Parent**(BlockID)
- **Child**(LocalID,BlockID)
  - 1≤LocalID≤8
- **Neigh**(FaceID, BlockID)
  - 1≤FaceID≤6
- **Rlevel**(BlockID)
- **Lbtype**(BlockID)
- **Flg_refine**(BlockID)

child(1, 2) = 9
child(2, 2) = 10
child(3, 2) = 11
⋮
child(8, 2) = 16

Local ID   Block ID

parent(9) = 2
parent(10) = 2
parent(11) = 2
⋮
parent(16) = 2

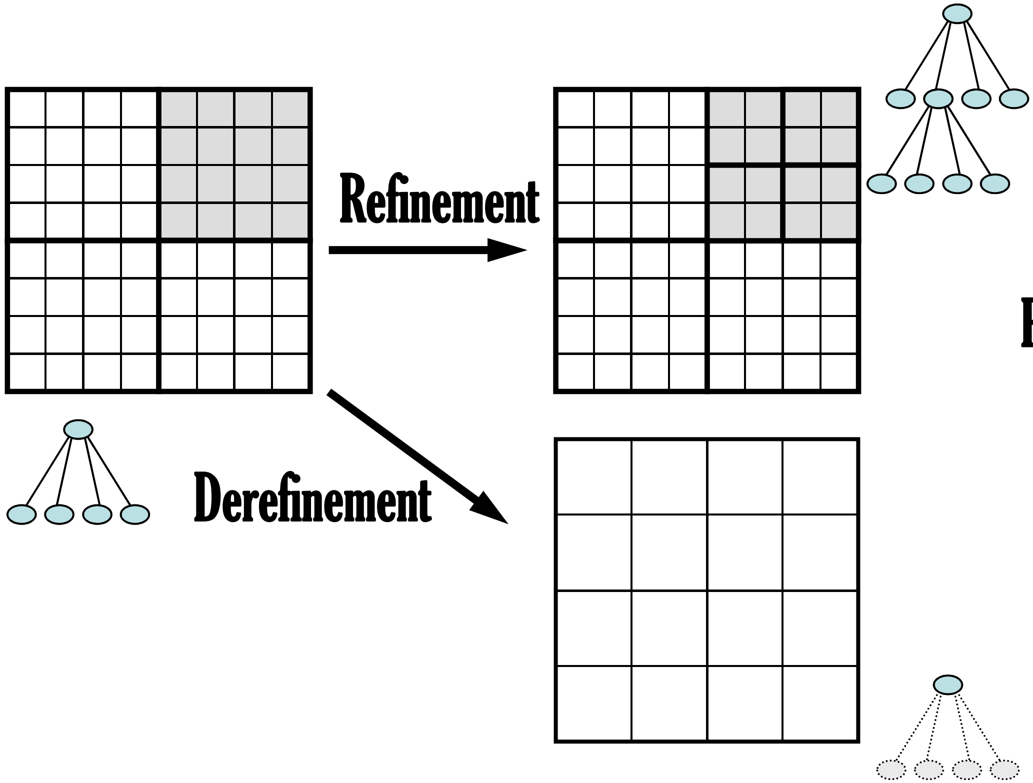
Block ID

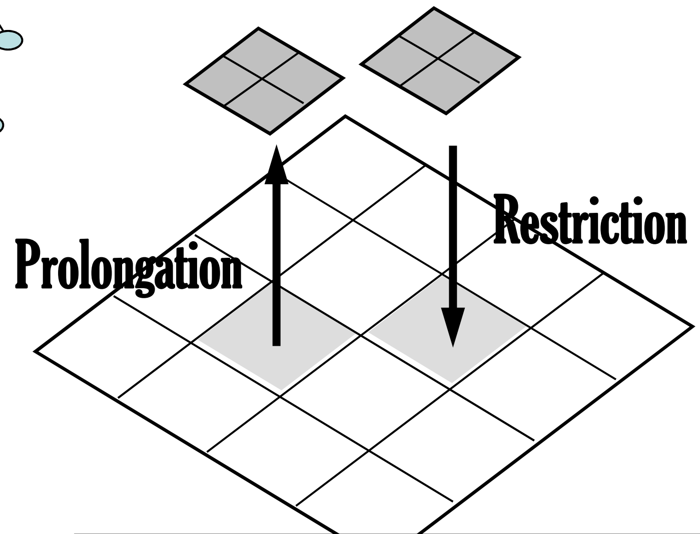
- If neighbors of a block include a physical boundary, any negative value is set there.
- If Lbtype=1, then the block is a leaf block, if =0, it has children.
- If Flag_refine=1, then refinement, =-1, derefinement, =0, no change.

Refinement/Derefinement

- **Refinement** — Interpolation/**Prolongation**
- **Derefinement** — Averaging/**Restriction**

A linear interpolation with limiter is used considering monotonicity preservation of the data across the boundary.

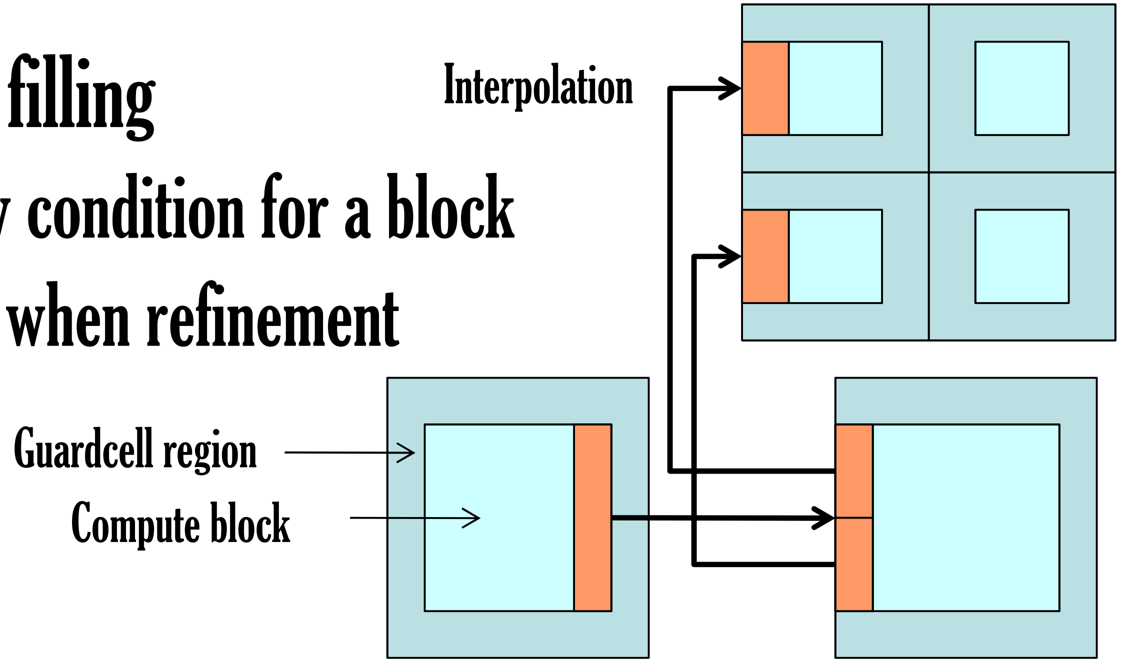




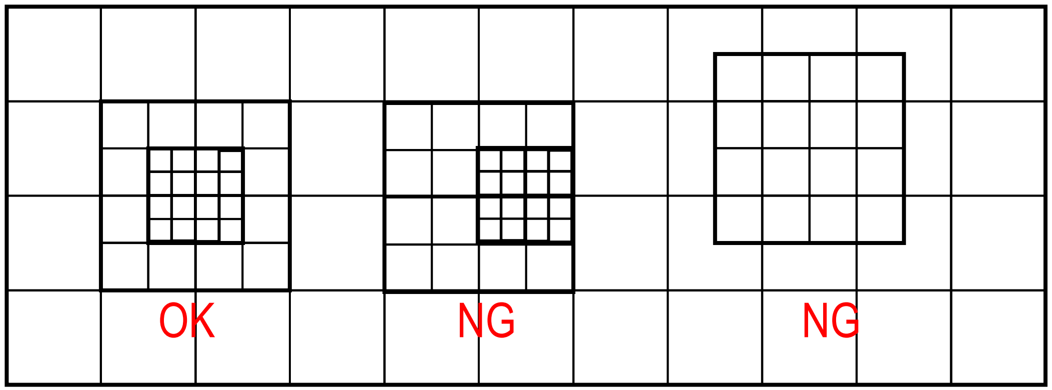
- Use physics-based refinement criteria, e.g. $\nabla\rho,\ \Delta M$
- Need experience for proper refinement
- Error estimation with Richardson extrapolation

Refinement/Derefinement(2)

- Guardcell (Ghostcell) filling
  - Used as the boundary condition for a block
  - Interpolation needed when refinement



- Proper nesting

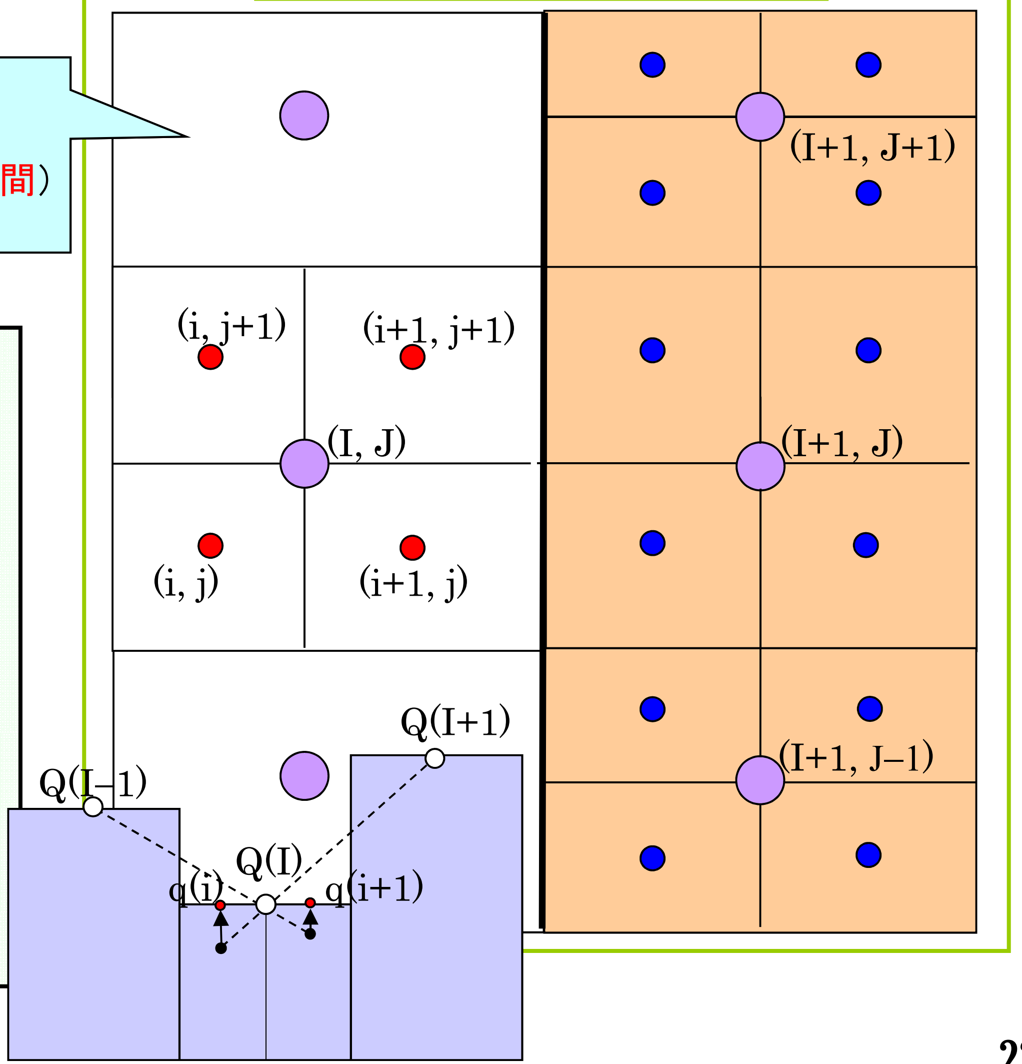


ブロック境界での内挿法

格子解像度が異なる接合面における線形補間
に単調性の維持を組み込む方法を採用

- 太線がブロック境界
- 青丸がレベルl+1格子のセル中心（未知）
- 赤丸がレベルl+1格子のガードセルの中心（要補間）
- 紫丸がレベルl格子のセル中心（既知）

ブロック境界付近の格子図



●のガードセル位置における内挿補間式

$$
\boxed{
\begin{aligned}
Q^{l+1}_{i,j} &= Q^{l}_{I,J} - 0.25\Delta_{\xi} - 0.25\Delta_{\eta},\\
Q^{l+1}_{i+1,j} &= Q^{l}_{I,J} + 0.25\Delta_{\xi} - 0.25\Delta_{\eta},\\
Q^{l+1}_{i,j+1} &= Q^{l}_{I,J} - 0.25\Delta_{\xi} + 0.25\Delta_{\eta},\\
Q^{l+1}_{i+1,j+1} &= Q^{l}_{I,J} + 0.25\Delta_{\xi} + 0.25\Delta_{\eta}
\end{aligned}
}
$$

where

$$\Delta_{\xi} = 0.5(sign(\Delta^{+}_{\xi}) + sign(\Delta^{-}_{\xi}))\min\left(\left|\Delta^{+}_{\xi}\right|, \left|\Delta^{-}_{\xi}\right|\right)$$

$$\Delta_{\eta} = 0.5(sign(\Delta^{+}_{\eta}) + sign(\Delta^{-}_{\eta}))\min\left(\left|\Delta^{+}_{\eta}\right|, \left|\Delta^{-}_{\eta}\right|\right)$$

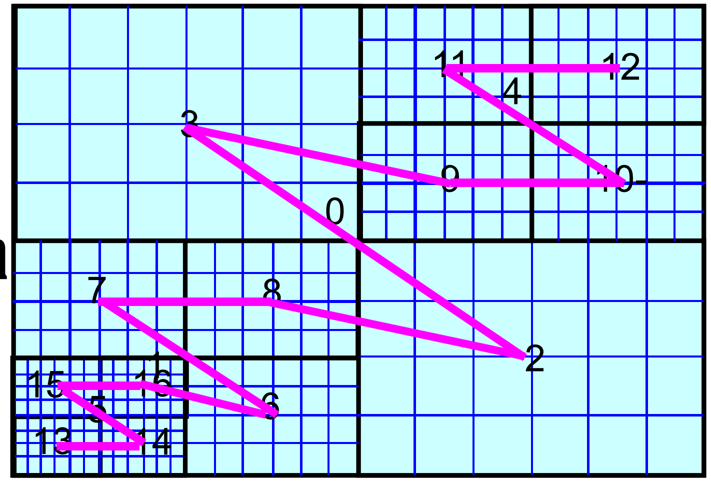
$$\Delta^{+}_{\xi} = Q^{l}_{I+1,J} - Q^{l}_{I,J},\ \Delta^{-}_{\xi} = Q^{l}_{I,J} - Q^{l}_{I-1,J}$$

$$\Delta^{+}_{\eta} = Q^{l}_{I,J+1} - Q^{l}_{I,J},\ \Delta^{-}_{\eta} = Q^{l}_{I,J} - Q^{l}_{I,J-1}$$

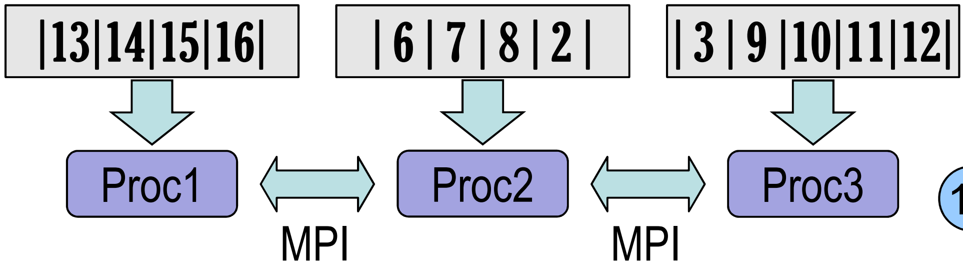
Parallelization and Load Balance

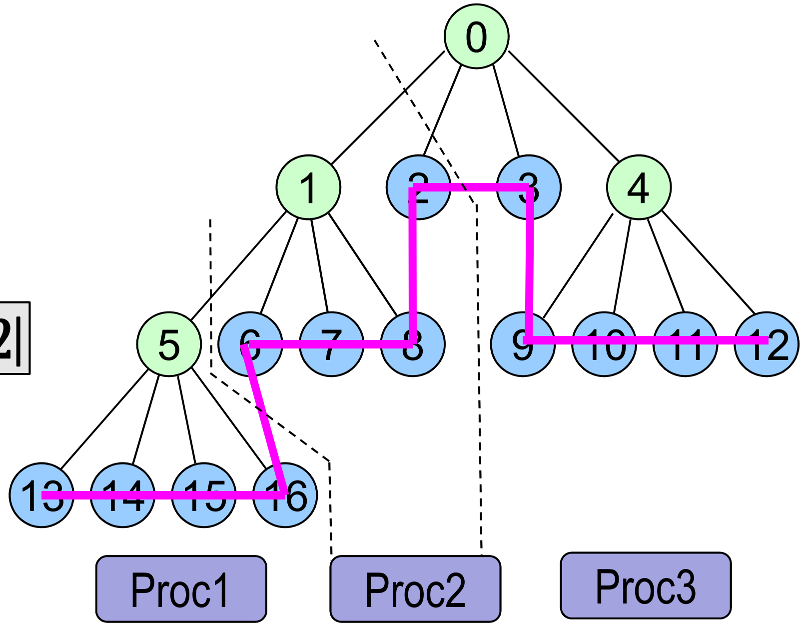
- **Space filling curve (Z-ordering)**
  - Assign 2D/3D blocks to a 1D ordering
  - Preserve locality >> Less communication

|13|14|15|16| 6 | 7 | 8 | 2 | 3 | 9 |10|11|12|

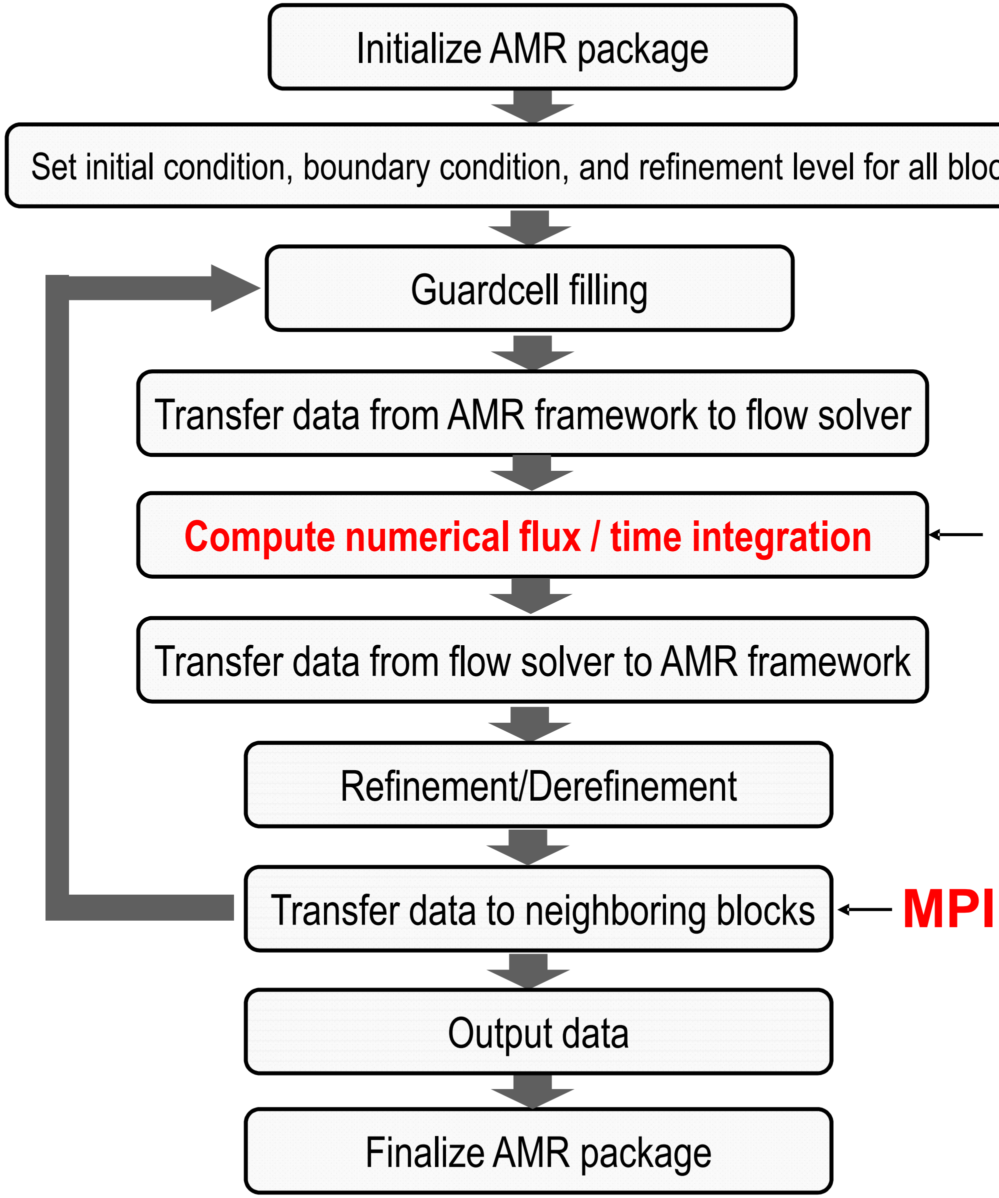


- **Domain-based partitioning**
  - For load balance
  - MPI only between processes



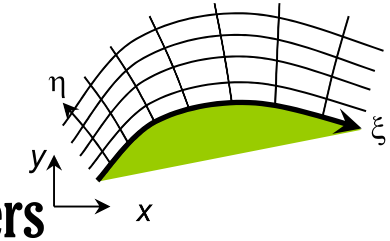


Code Structure

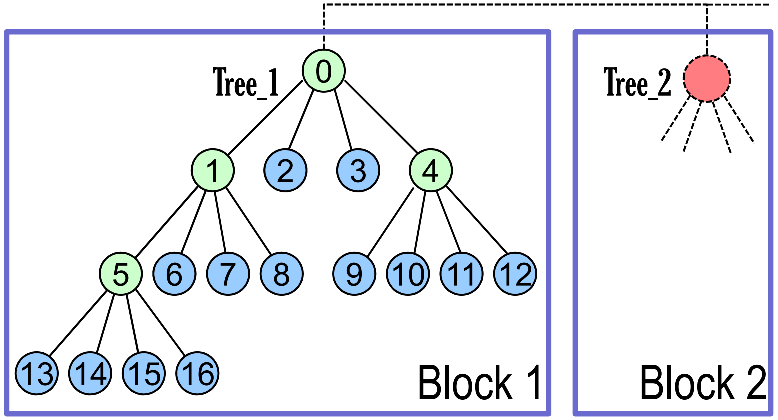


- Separate the AMR framework completely from the kernel solver
- Written by Fortran90 using module, allocatable array, etc.
- No pointer, no structure element , considering compute performance

Additional Implementations for Practical Use



- Introduce **body-fitted curvilinear coordinate system**
  - Allow for anisotropic mesh, treat thin boundary and shear layers
- Use **efficient initial block** assignment
  - Multiple roots
- Reduce and optimize **memory usage**
  - A process has only related local arrays
- Reduce and optimize **MPI communication**
  - Communicate only guardcell data among blocks

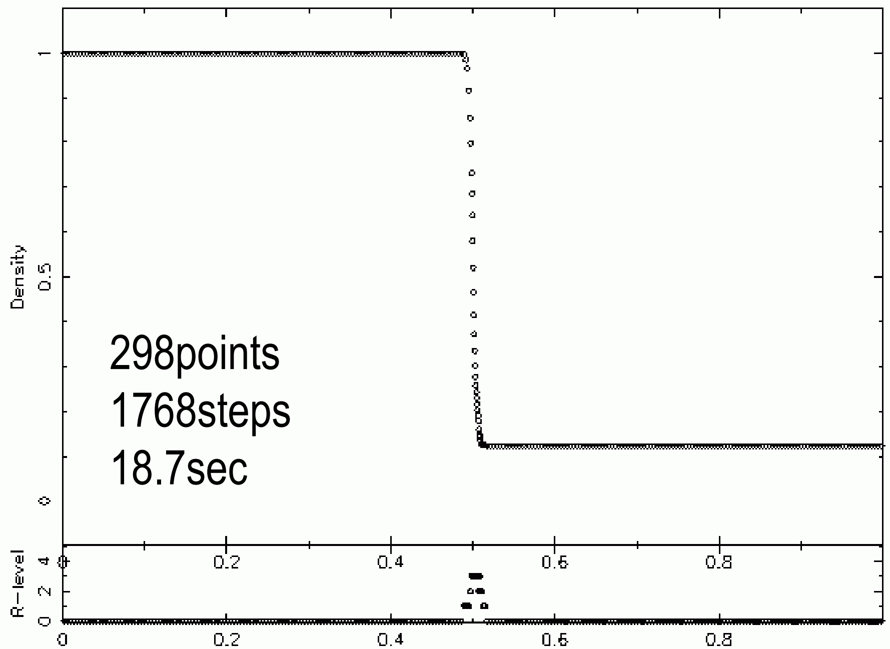


Kernel Solver for Single Grid

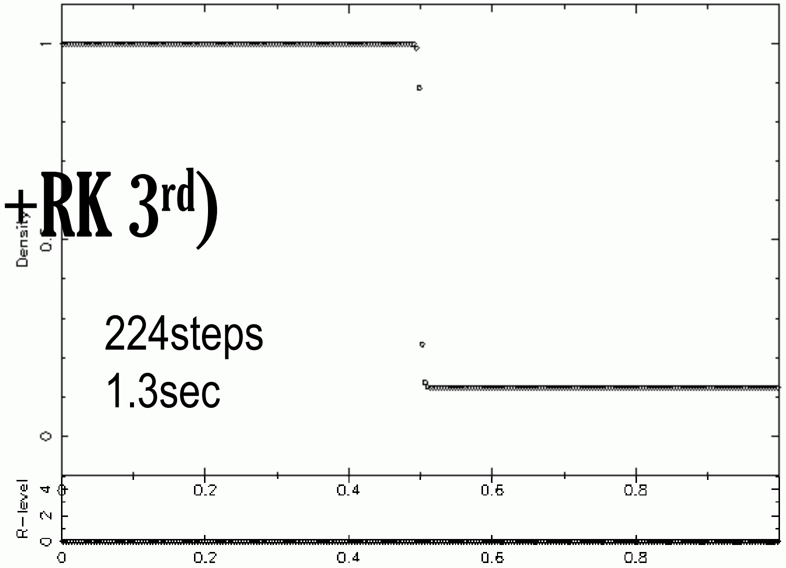
- Governing equations
  - 2D/3D Compressible Navier-Stokes for perfect gas
- Numerical method
  - Spatial discretization
    - Finite volume approach
    - Roe/AUSM numerical flux with MUSCL/WENO interpolation
  - Time integration
    - Implicit LUADI or Explicit Runge-Kutta

1D Shocktube

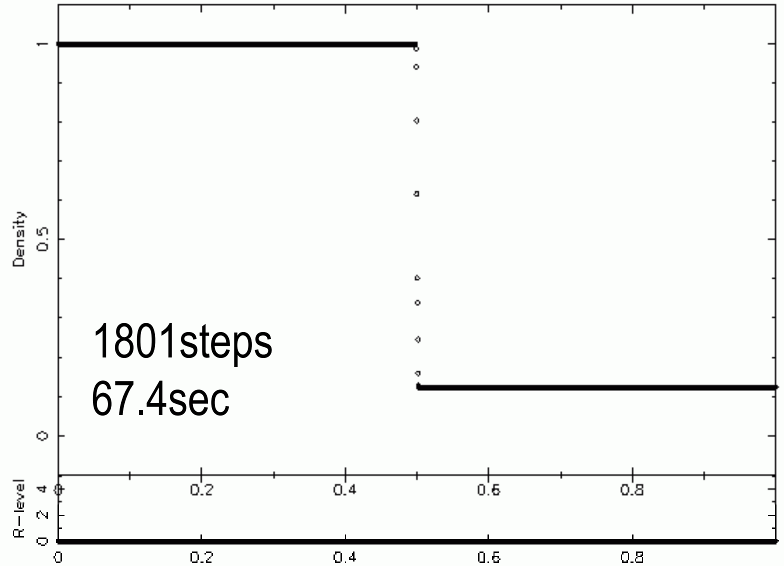
- Sod's standard problem (Weno 5^{th}-Roe+RK 3^{rd})



With AMR (Rlevel=3)



Without AMR (uniform 256 points)

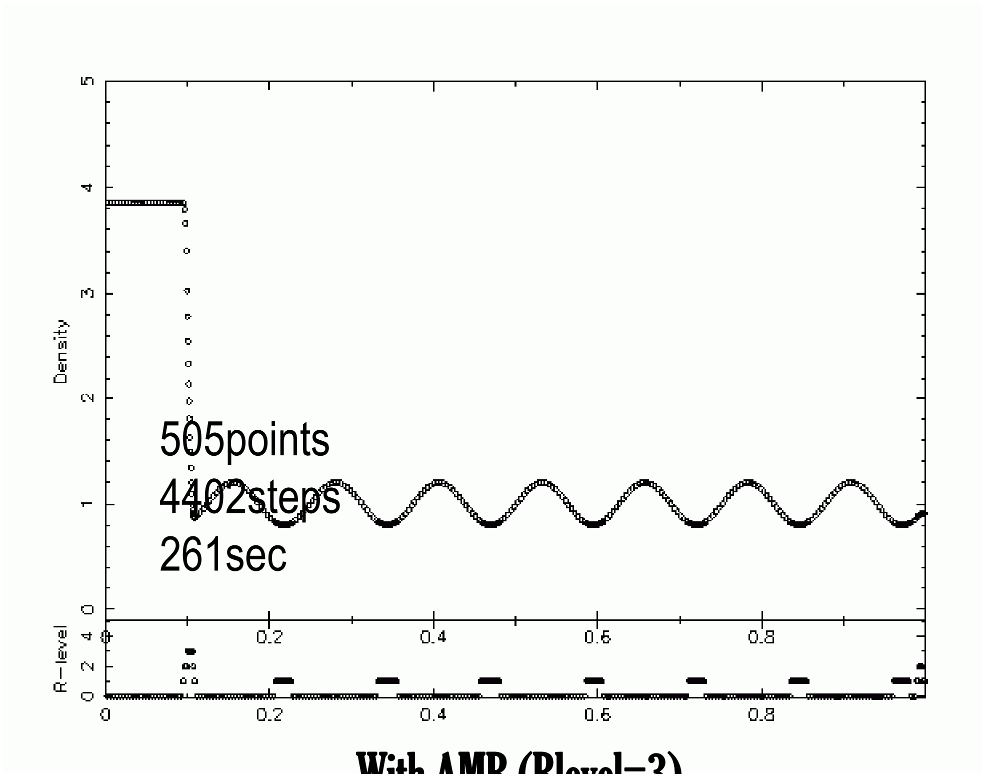


Without AMR (uniform 2,048 points)

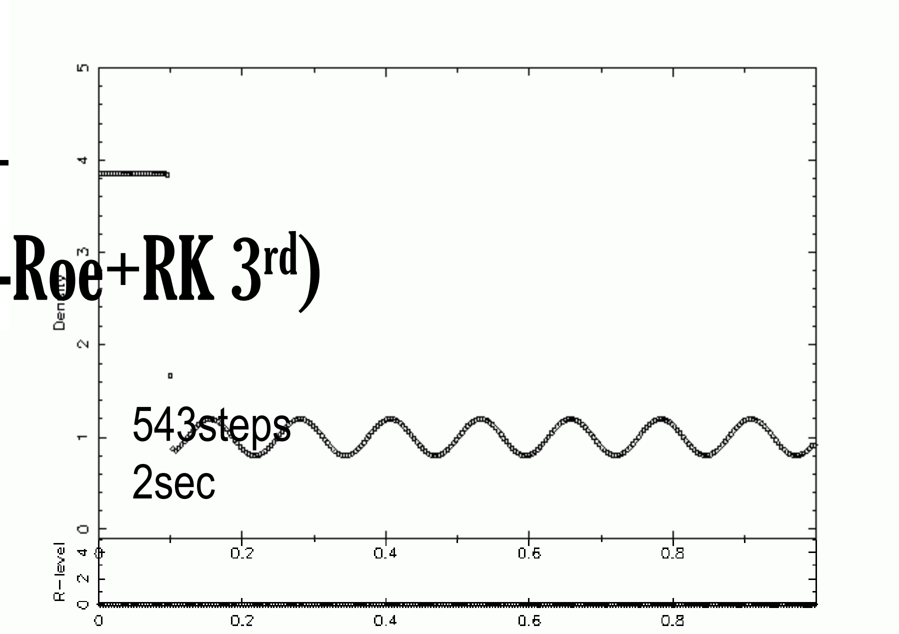
- CPU Time : 256pts < AMR < 2,048pts
- Shock becomes steepened
- Contact surface remains with initial gradient

1D Shocktube(2)

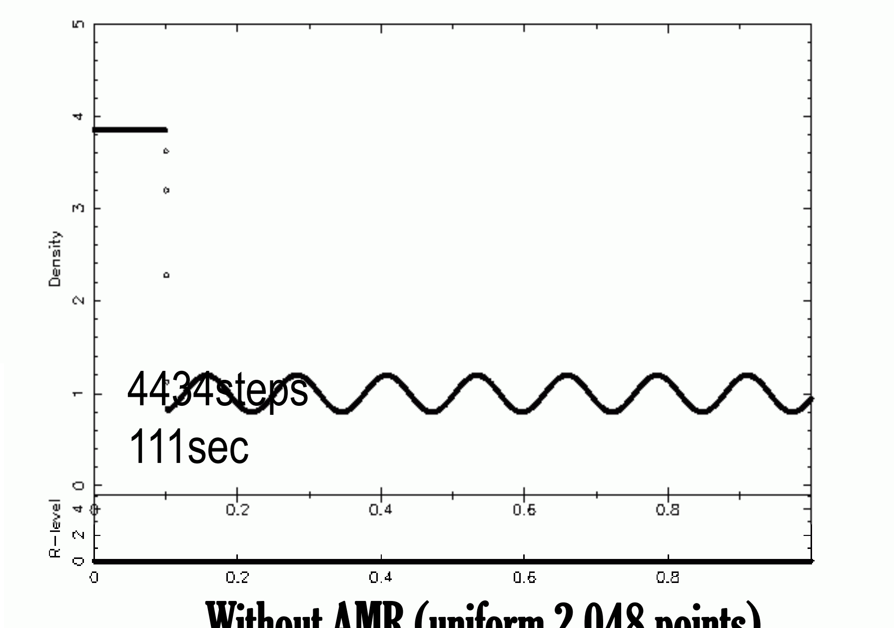
● Shu-Osher's entropy wave (Weno 5th-Roe+RK 3rd)



With AMR (Rlevel=3)



Without AMR (uniform 256 points)

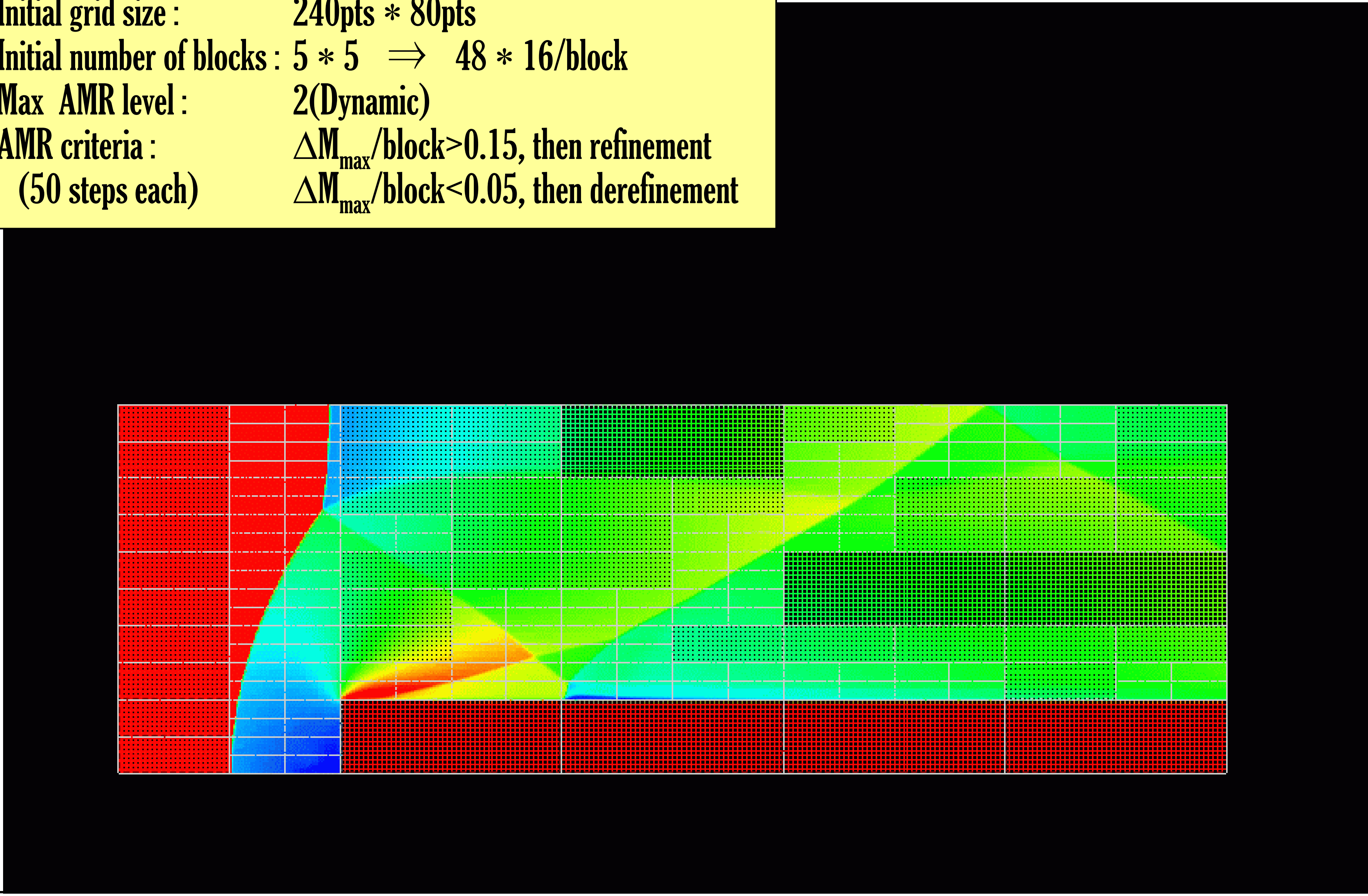


Without AMR (uniform 2,048 points)

- AMR is useful for capturing complex waves
- AMR consumes more CPU time than expected

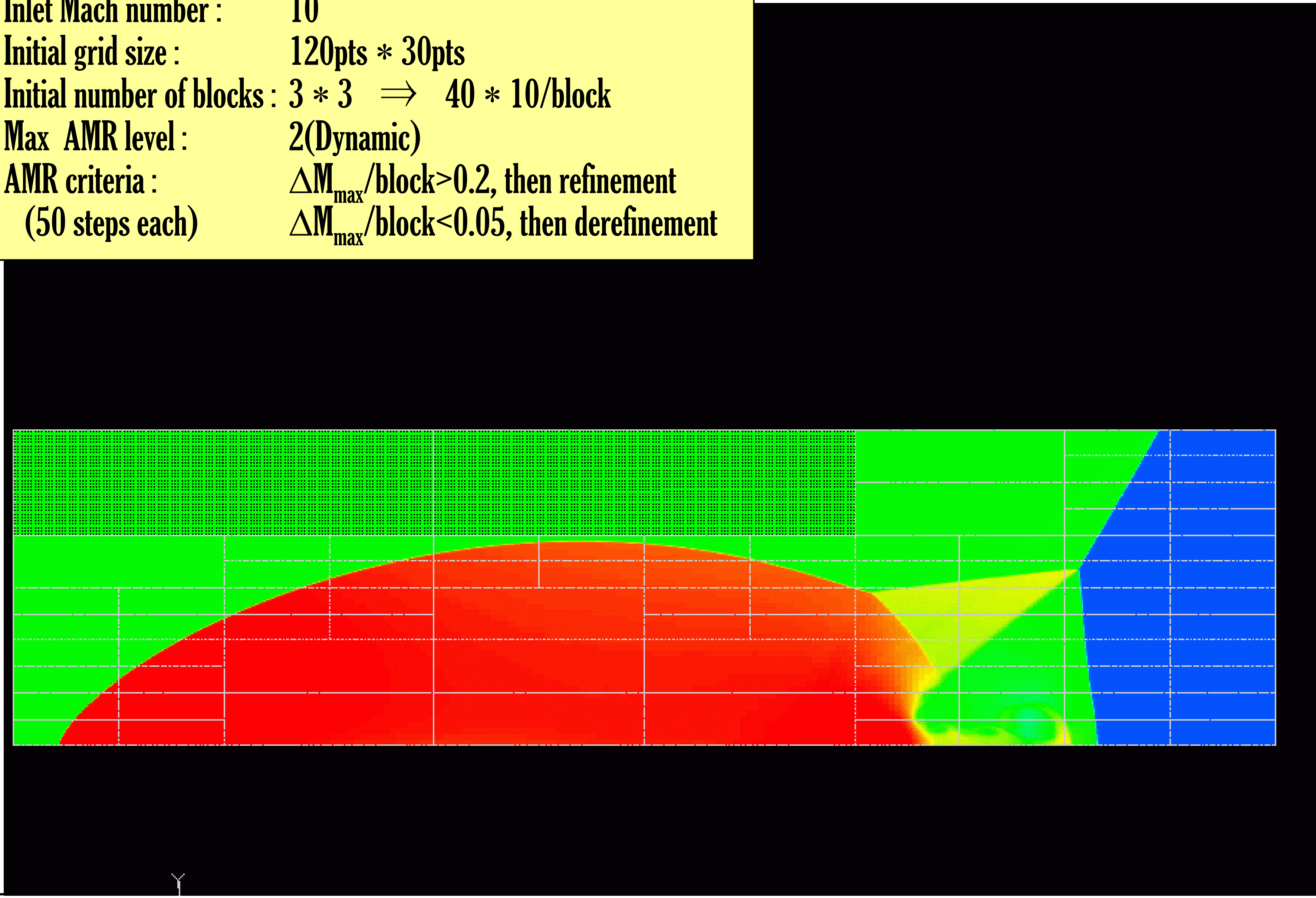
2D Forward Step

Inlet Mach number : 3
Initial grid size : 240pts $*$ 80pts
Initial number of blocks : 5 $*$ 5 $\Rightarrow$ 48 $*$ 16/block
Max AMR level : 2(Dynamic)
AMR criteria : ΔM_{max}/block>0.15, then refinement
(50 steps each) ΔM_{max}/block<0.05, then derefinement

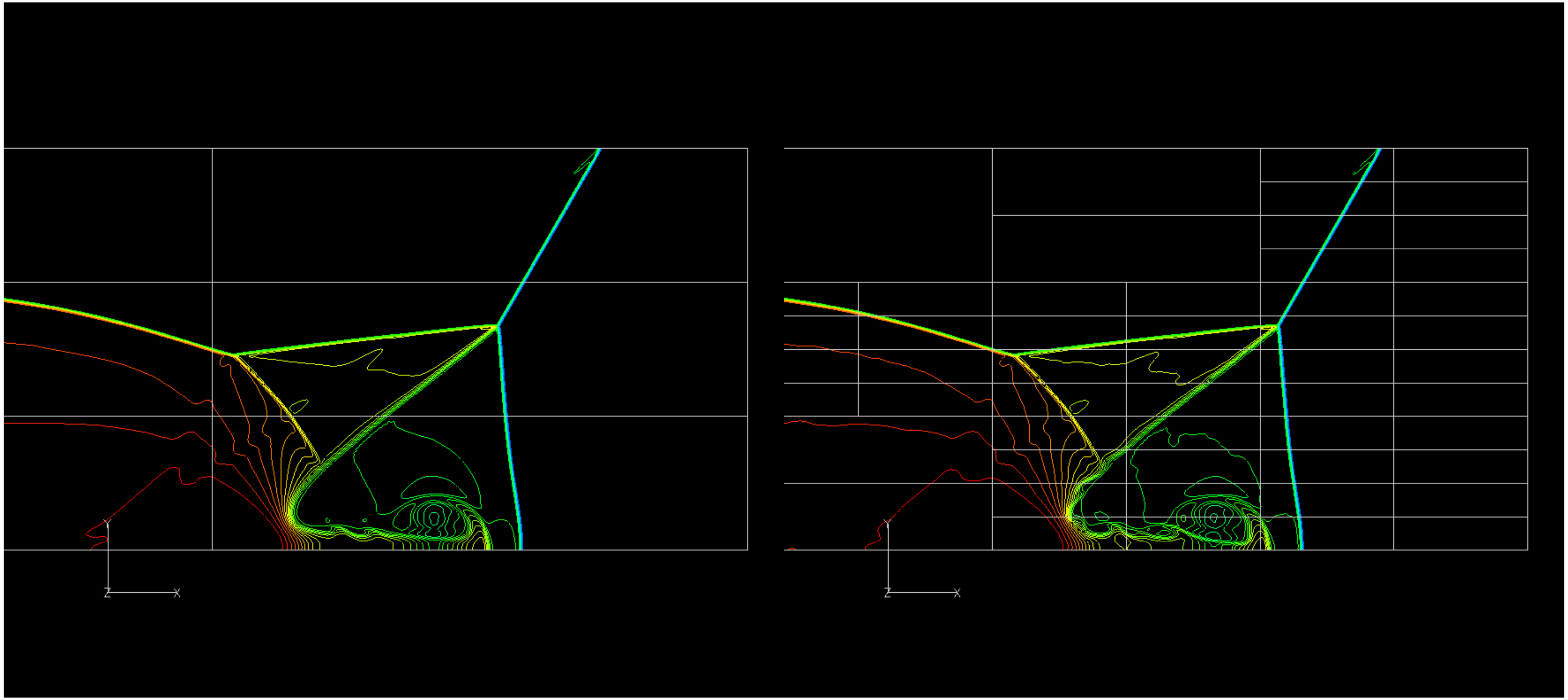


2D Double Mach Reflection

Inlet Mach number : 10
Initial grid size : 120pts $*$ 30pts
Initial number of blocks : 3 $*$ 3 $\Rightarrow$ 40 $*$ 10/block
Max AMR level : 2(Dynamic)
AMR criteria : ΔM_{max}/block>0.2, then refinement
(50 steps each) ΔM_{max}/block<0.05, then derefinement



2D Double Mach Reflection(2)



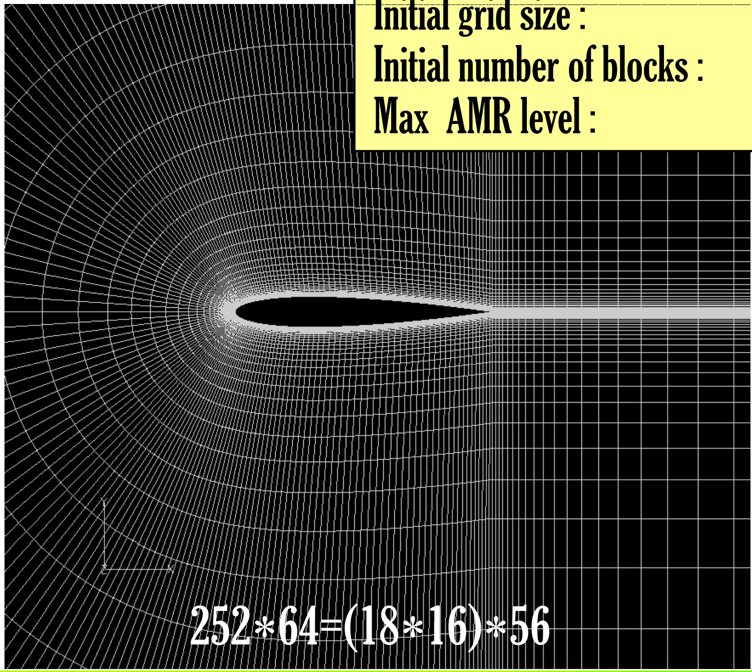
Without AMR, uniform 1920 ∗ 480

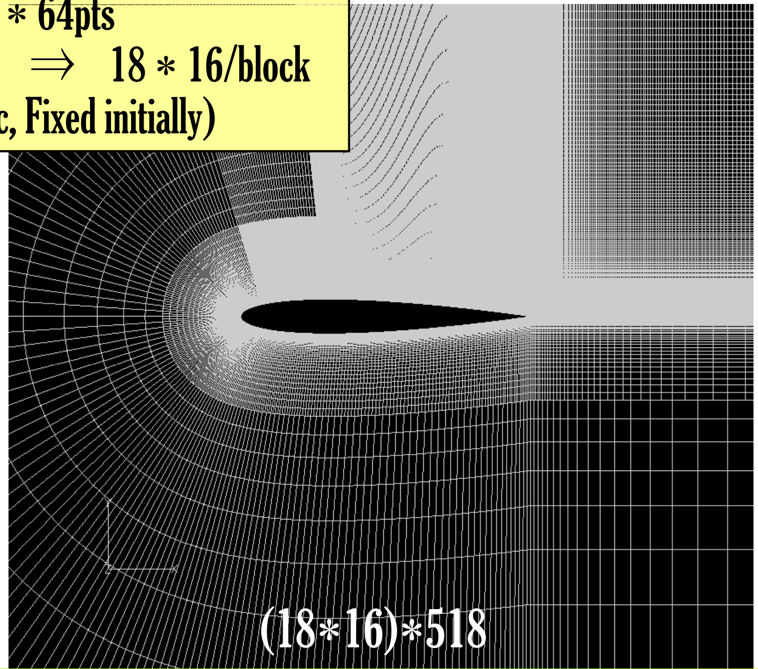
With AMR, initial 480 ∗ 120 and Rlevel=2

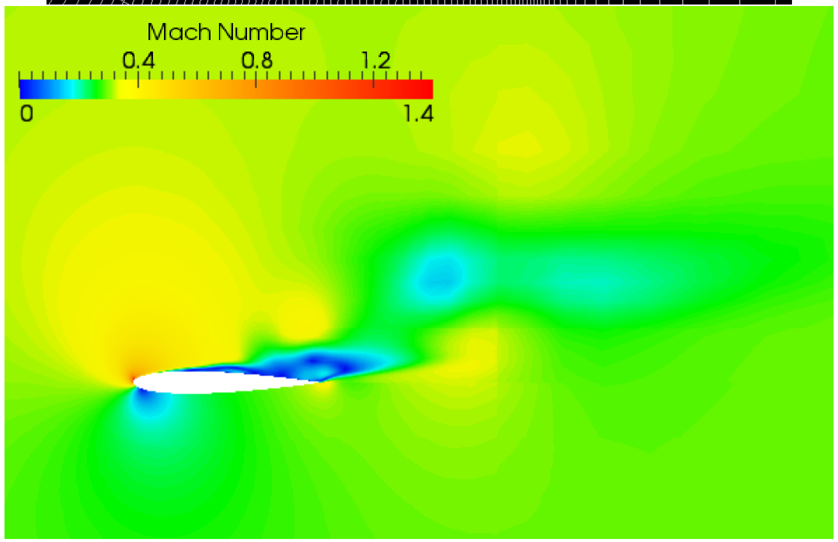
Almost same resolution can be obtained locally with/without AMR.

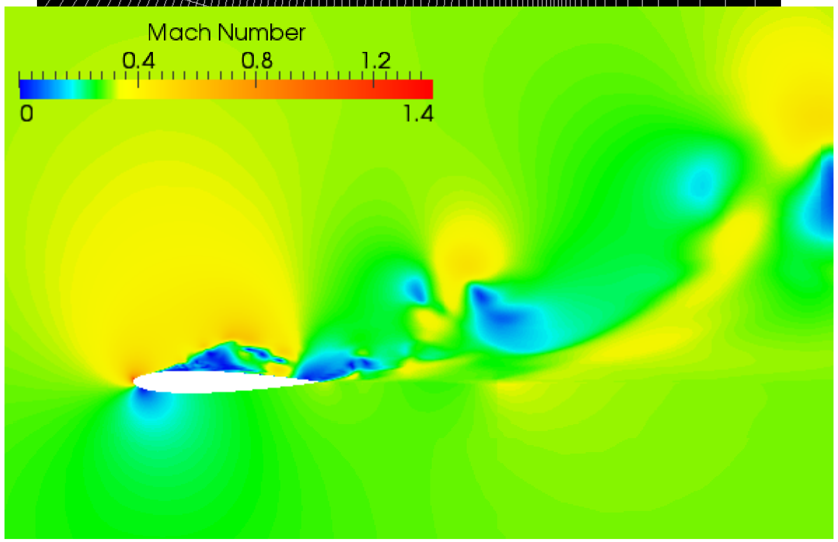
2D Airfoil

Mach number :	0.3
Angle of attack:	20degree
Reynolds number:	$1.0 * 10^6$
Initial grid size :	252pts * 64pts
Initial number of blocks :	14 * 4 ⇒ 18 * 16/block
Max AMR level :	3(Static, Fixed initially)



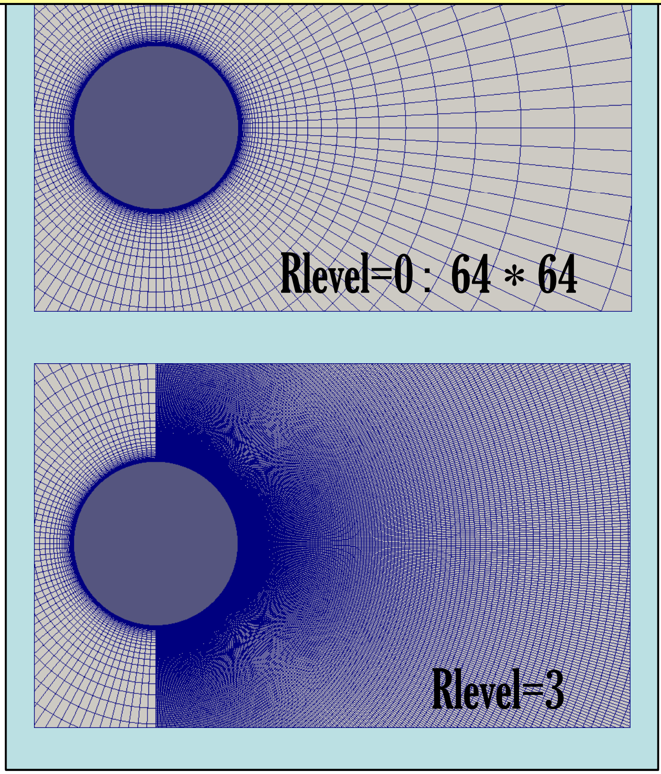




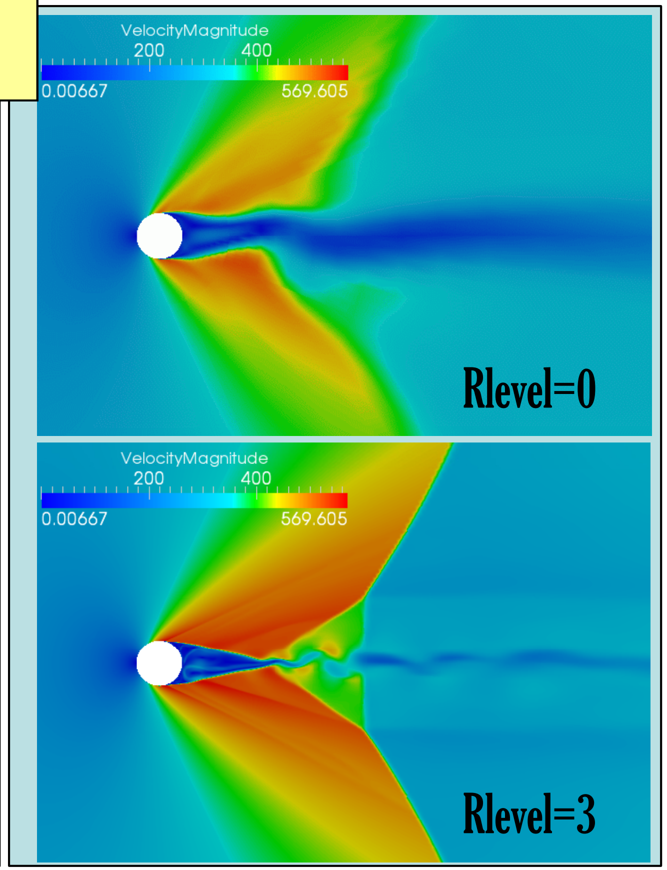


2D Circular Cylinder

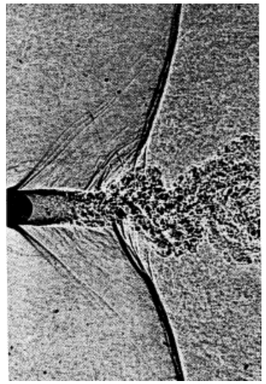
Mach number : 0.95
Reynolds number: $1.35 * 10^6$
Initial grid size : 64pts * 64pts
Initial number of blocks : $3 * 3 \Rightarrow 40 * 10$/block
Max AMR level : 3(Static, Fixed initially)



Grid

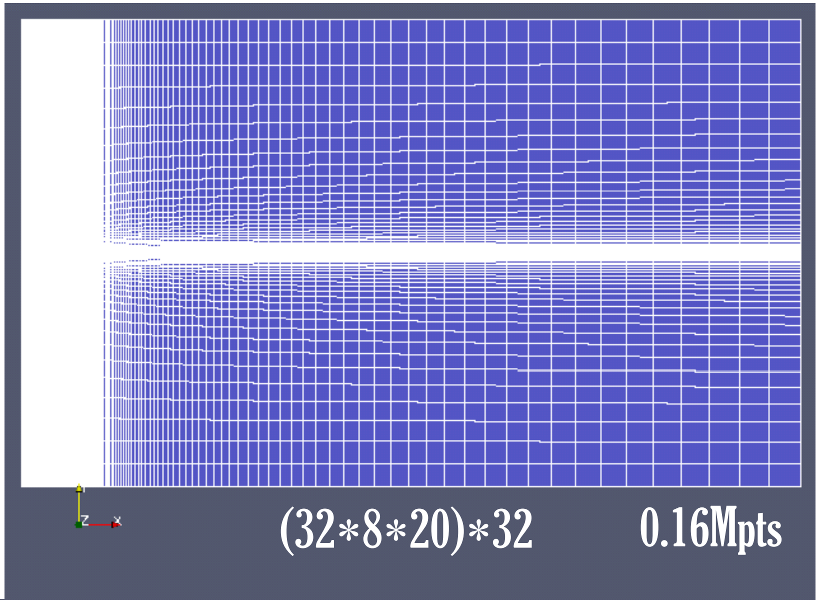


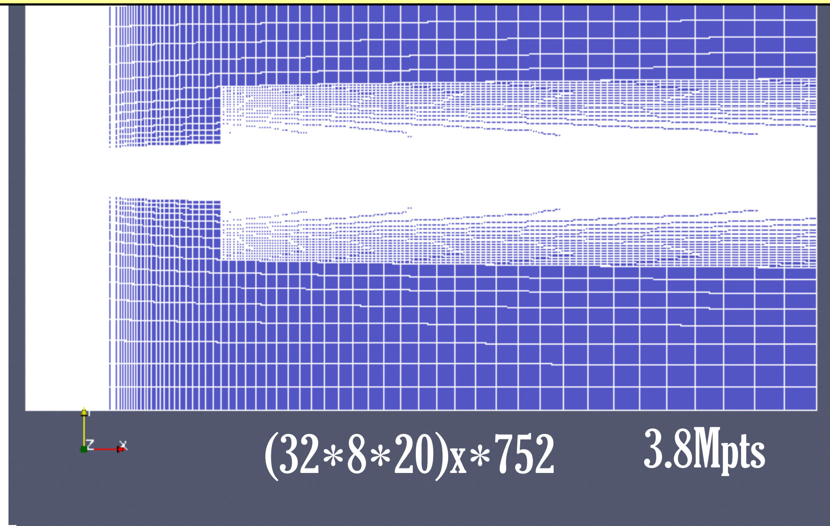
Snapshot of the velocity magnitude

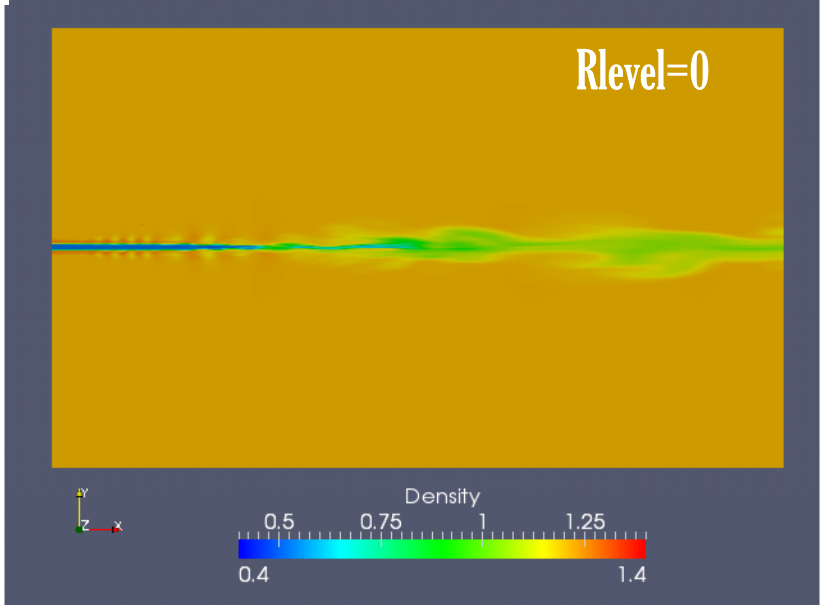

Experiment

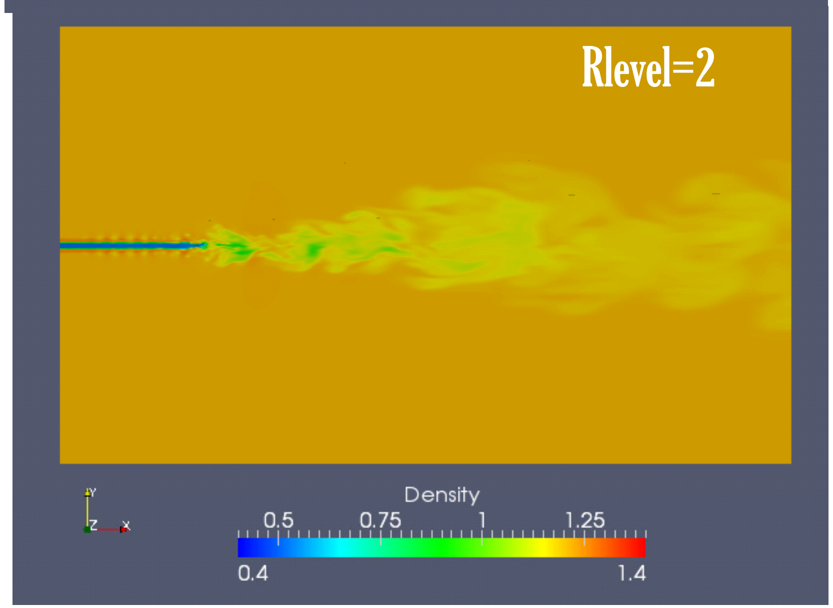
3D Supersonic Coaxial Jet

Mach number :	M_{core}=0.76, M_{fan}=0.58
Reynolds number:	Re= $5 * 10^6$
Initial grid size :	128pts * 32pts * 40pts
Initial number of blocks :	$4 * 4 * 2 \Rightarrow 32 * 8 * 20$/block
Max AMR level :	2(Static, Fixed initially)



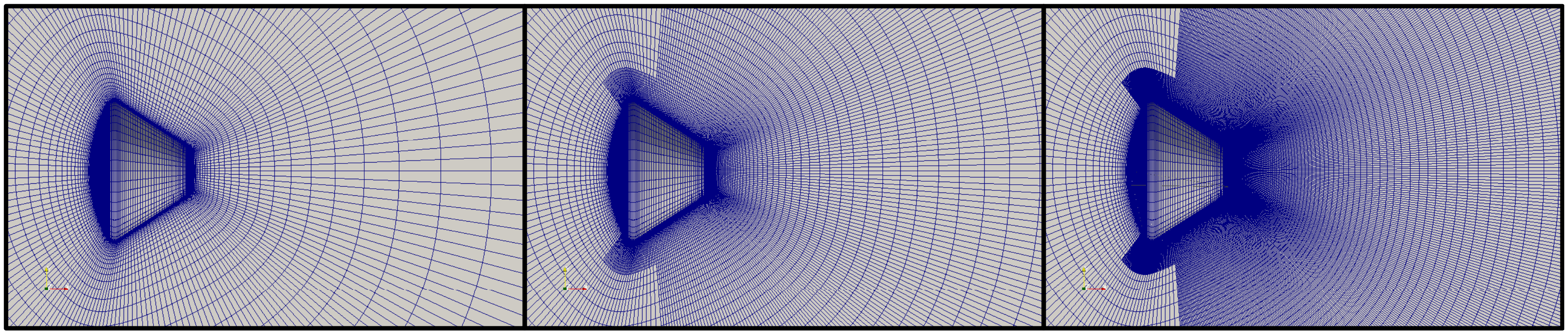






3D Atmospheric Reentry Capsule

- HTV-R first flight from ISS is expected around 2017.
- Here, ORION CM is studied to investigate transonic unsteady flow phenomena behind reentry capsule.

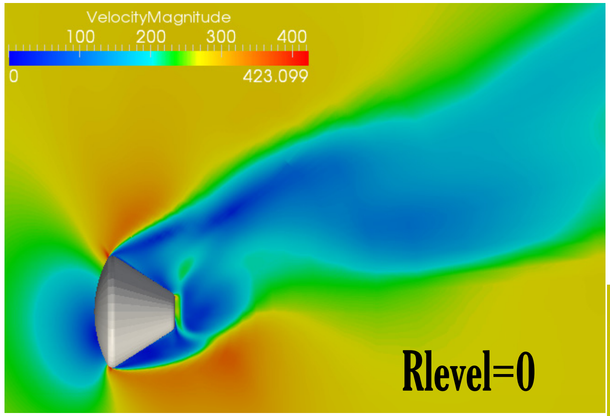


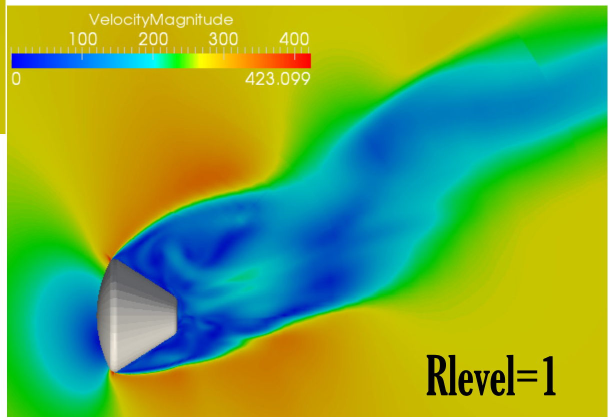
Rlevel=0 Rlevel=1 Rlevel=2

3D Atmospheric Reentry Capsule(2)

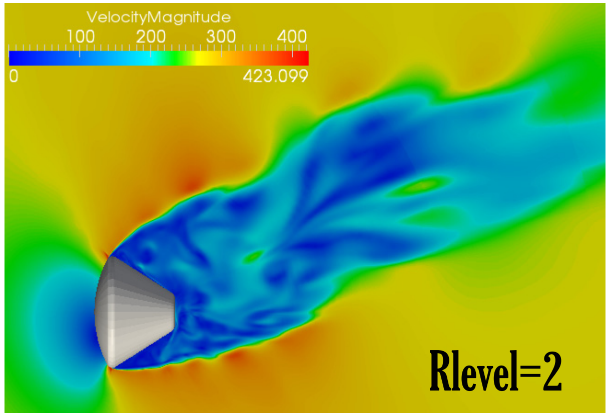
- Time-dependent unsteady flow fields

Mach number :	0.8
Angle of attack:	20degree
Reynolds number:	$1.2 * 10^7$
Initial grid size :	96pts * 60pts * 40pts
Max AMR level :	2(Static, Fixed initially)





$\Delta t = 0.145 * 10^{-5}$ (CFL~100)
20,000 steps computed by ILES
(10hrs/32CPU@JSS)
Movie: snapshot every 500 step



As the refinement level enhances, fine scale vortical structures can be captured in the separated region behind the capsule.

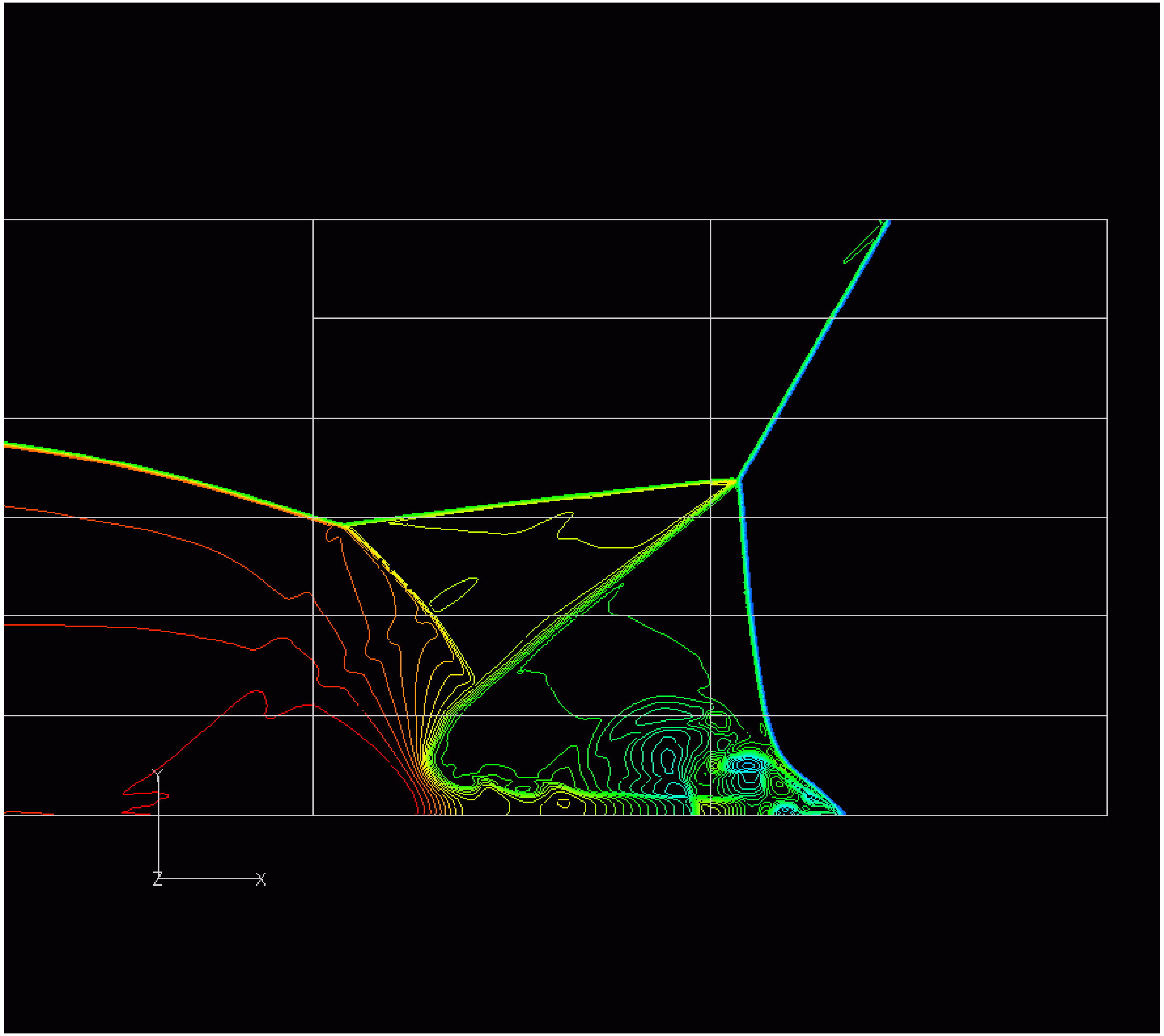
Summary and Future Work

- The AMR framework based on structured mesh is depicted, and the extension for its practical usage is shown.
- It is found that the AMR is effective to clearly capture complex fluid flow phenomena with less grid points in total.
- It is shown that the AMR framework could be used to the practical aerodynamic problems at JAXA.
- Future work is associated with the completion of the AMR basic functions not yet implemented, and further V&V.

実務における数学的課題

- カーバンクルの撲滅
  - 離散モデルと連続の整合性
- 精度評価，誤差評価
  - 非構造格子ソルバーにおける高精度化
  - 格子品質の数学的評価
- 時間積分法
  - ルンゲクッタは時間がかかりすぎる
- 大規模問題
  - 行列解法の収束加速

Entropy fixを適用しない場合のカーバンクル



超音速流における問題