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地球規模流動現象解明のための計算科学
大規模数値シミュレーション

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流動現象の自由度

乱流現象の自由度：$O(Re^{9/4})$　（Re：レイノルズ数）

	Re	自由度
歩行(4km/h, L=0.5m)	3.70×10^{4}	1.9×10^{10}
自転車(20km/h, L=0.5m)	1.85×10^{5}	7.1×10^{11}
自動車(60km/h, L=2.0m)	2.22×10^{6}	1.9×10^{14}

空気の動粘性係数：$\nu=1.5\times10^{-5}\mathrm{m^2/s}$

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流動現象の大規模数値シミュレーション

レイノルズ数10^4の流動現象の数値シミュレーション

↓

格子点数：10^9点
（１自由度／１格子点）

↓

最低32GbyteのMemory

8Gbyte／変数（倍精度）×4変数（速度3，圧力1）

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流動現象の大規模数値シミュレーション

ハードウェア性能

- **Memory容量：最低32Gbyte**
- **Disk容量：数百Gbyte～数Tbyte**
- **CPUアーキテクチャ：シングル or パラレルCPU**

シングルCPU & 32Gbyte Memory

→ 非現実的

パラレルCPU & 32Gbyte Memory

→ 現実的

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流動現象の大規模数値シミュレーション

ソフトウェア

- パラレル**CPU**：理論的に**CPU**台数倍の
  スピードアップ可能

→ パラレル・アーキテクチャに
適合したスキーム

- パラレル化

→ 自動パラレル化：コンパイラ未成熟
手動パラレル化：**MPI，PVM**等の
Message Passing Library

流動現象の大規模数値シミュレーション

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プラットフォーム

流動現象数値シミュレータ

Exemplar V-class (HP)

3 Hyper-nodes
Processor : PA8200 (200MHz)
32PU : 16 , 8 , 8PU
48Gbyte : 16 , 16 , 16Gbyte

Hyper-node内：共有メモリ
Hyper-node間：分散メモリ

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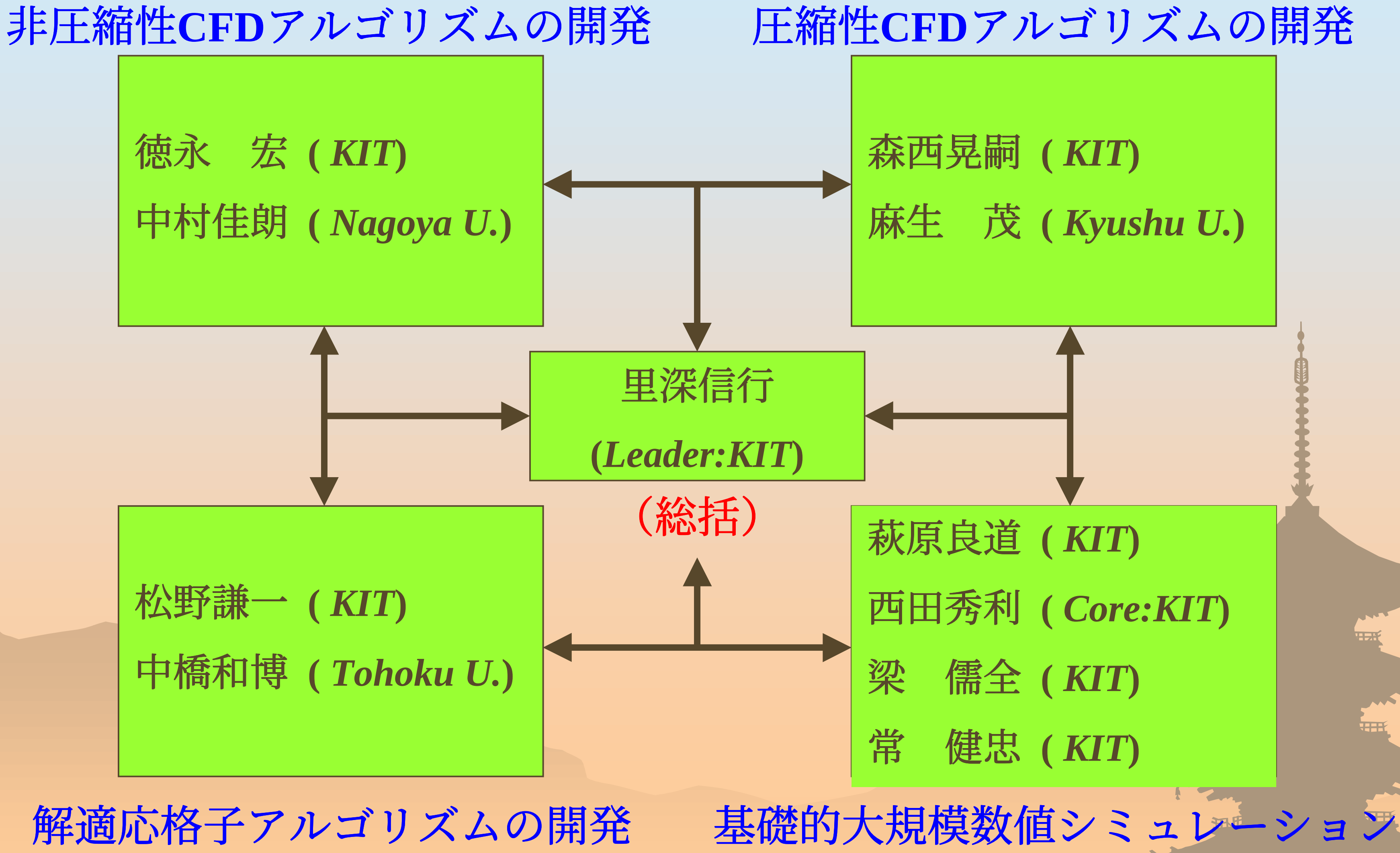
研究組織



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研究計画概要

- 超並列型コンピュータ適合計算流体力学アルゴリズムの開発
  - *高次精度線の方法*
  - *格子ボルツマン法*
- 超並列型コンピュータ適合解適応格子生成アルゴリズムの開発
  - *分解能向上*
- 基礎的大規模数値シミュレーション
  - *立方化球座標系*
  - *仮想境界デカルト格子法*
  - *コリオリ力，密度成層効果*

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Higher Order Method of Lines

Incompressible Navier-Stokes Equations

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_i^2}$$

Spatial Discretization:

Variable Order Proper Convective Scheme
Modified Differential Quadrature Method

$$\frac{d\vec{u_i}}{dt} = \vec{W}_i(\vec{u_i})$$

Time Integration:

3rd or 4th Order Runge-Kutta Scheme

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Modified Differential Quadrature (MDQ) Method

$$\frac{\partial u}{\partial x}\Big|_k \cong \sum_{m=-M/2}^{M/2} a_{k,m} u_{k+m} \qquad \frac{\partial^2 u}{\partial x^2}\Big|_k \cong \sum_{m=-M/2}^{M/2} b_{k,m} u_{k+m}$$

M: Order of Spatial Accuracy

$$a_{k,m} = \frac{\Pi'(x_k)}{(x_k - x_{k+m})\Pi'(x_k)} \qquad b_{k,m} = \sum_{l=-M/2}^{M/2} a_{k,l}\, a_{l,m}$$

$$a_{k,0} = \Pi''(x_k)/2\Pi'(x_k)$$

$$\Pi(x) = (x - x_{k-M/2})\ldots(x - x_k)\ldots(x - x_{k+M/2})$$

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Variable Order Proper Convective Scheme

$$u_j \frac{\partial u_i}{\partial x_j}\Big|_k \cong \sum_{l=1}^{M/2} c_{l'} \overline{\overline{u_j}^{x_j} \frac{\delta_{l'} u_i}{\delta_{l'} x_j}}^{l' x_j} \qquad (l' = 2l - 1)$$

M: Order of Spatial Accuracy

$$\overline{u_j}^{x_j}\Big|_{k \pm l'/2} = \sum_{m=1}^{M/2} c_{m'} \frac{1}{2}\left[u_j \big|_{k \pm (l'+m')/2} + u_j \big|_{k \pm (l'-m')/2} \right]$$

$$\overline{\phi}^{l' x_j}\Big|_k = \frac{1}{2}\left(\phi_{k+l'/2} + \phi_{k-l'/2} \right)$$

$$\frac{\delta_{l'} u_i}{\delta_{l'} x_j}\Big|_{k \pm l'/2} = \frac{\pm 1}{l' h_{x_j}} \left(u_i \big|_{k \pm l'} - u_i \big|_k \right)$$

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Pressure Equation Solver

Variable Order Multigrid Method

$$\nabla^2 p^{n+1}|_k = \frac{1}{\Delta t}\frac{\partial \overline{u_i *}^{x_i}}{\partial x_i}|_k$$: Elliptic Equation

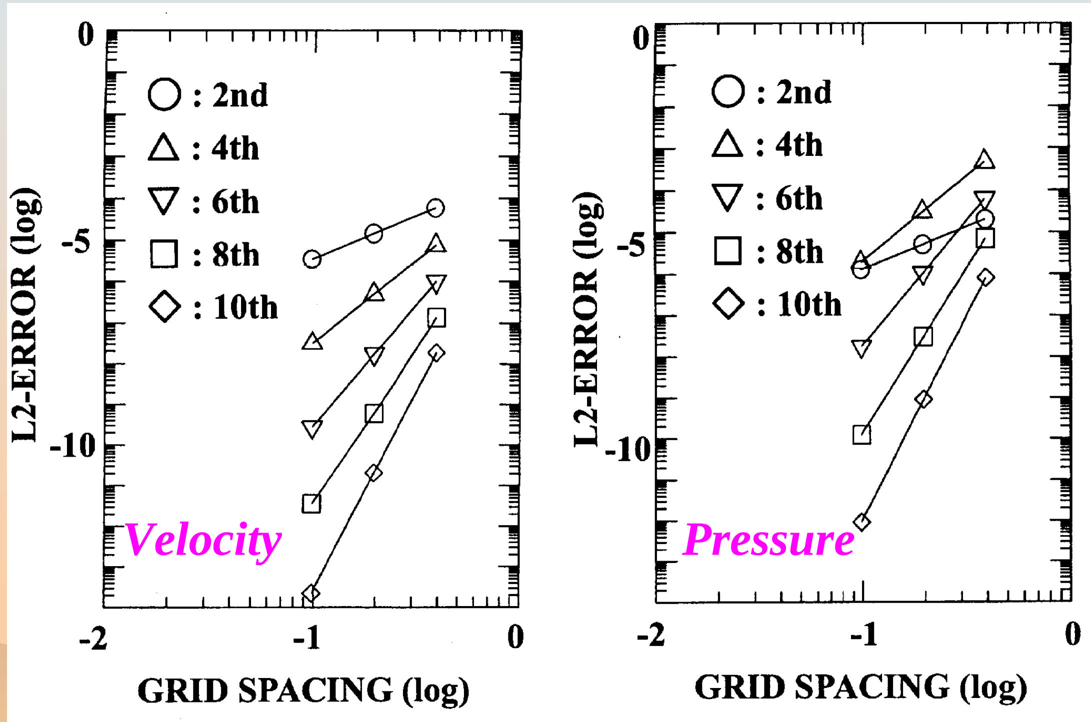
Unsteady Term (τ: Pseudo-time)

$$\frac{\partial p}{\partial \tau} = \nabla^2 p^{n+1}|_k - \frac{1}{\Delta t}\frac{\partial \overline{u_i *}^{x_i}}{\partial x_i}|_k$$: Parabolic Equation

- Higher Order Method of Lines
- Multigrid Method

Higher Order Method of Lines

Validation of Spatial Accuracy

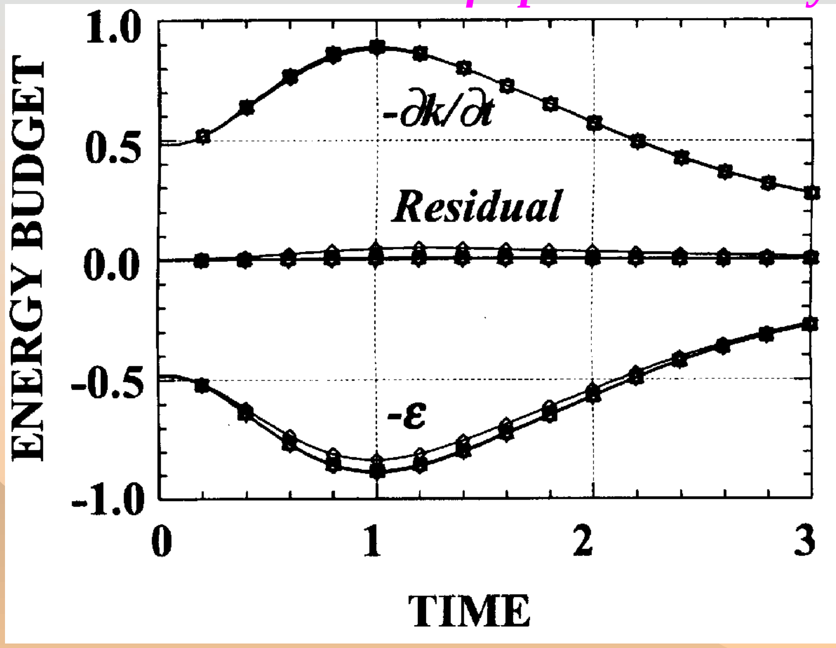


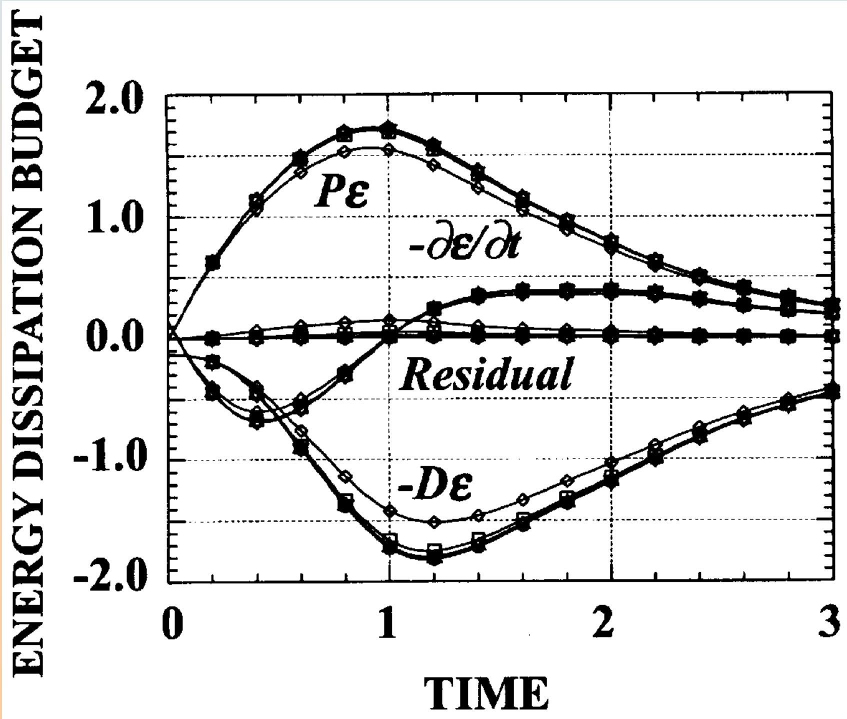
L2-Ratio

DNS of 3D Homogeneous Isotropic Turbulence Using Higher Order Method of Lines

Validation of Conservation Property

◇,□,△,▽,○ : 2nd, 4th, 6th, 8th, 10th Order of Spatial Accuracy





Energy and Energy Dissipation Budgets

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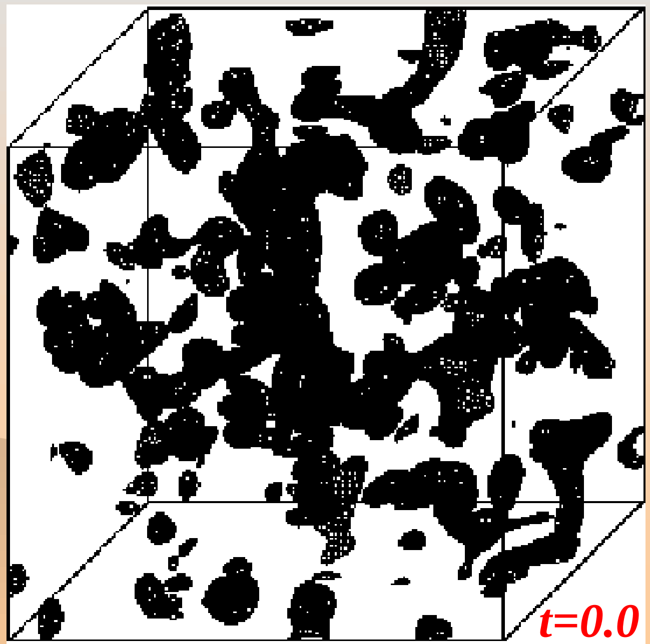
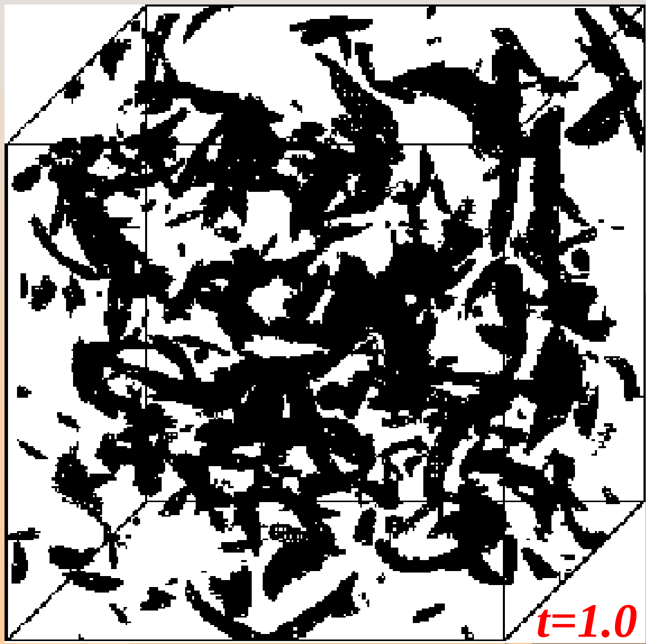
DNS of 3D Homogeneous Isotropic Turbulence Using Higher Order Method of Lines

Computational Conditions: 256^3 grid points
ν=1/1000 (Re_t=13800)
10th order of spatial accuracy





Iso-Surface of Enstrophy

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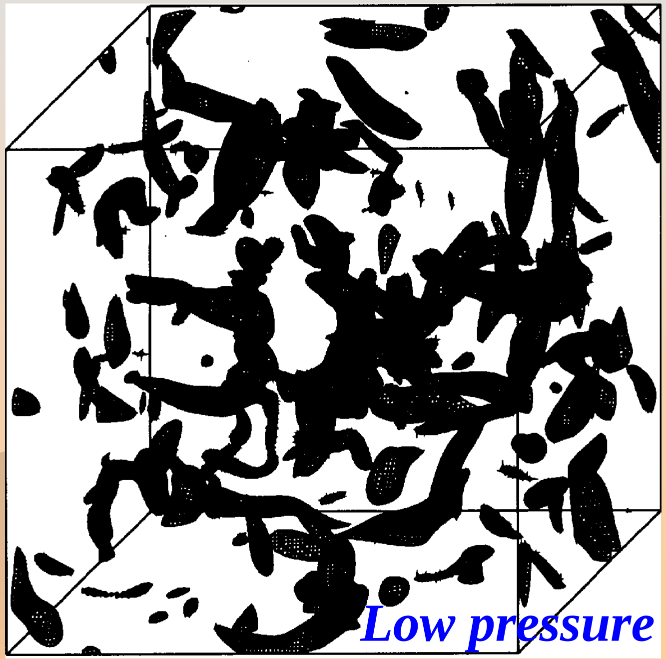
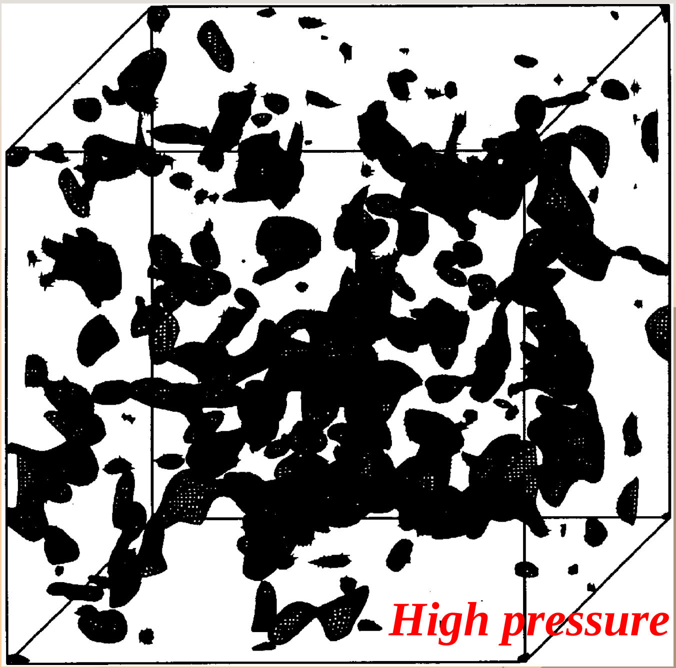
DNS of 3D Homogeneous Isotropic Turbulence Using Higher Order Method of Lines

Computational Conditions: 256^3 grid points
ν=1/1000 (Re_t=13800)
10th order of spatial accuracy





Iso-Surface of Pressure (t=1.0)

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Parallelization

Higher Order Method of Lines

Speedup Ratio : T(1)/T(pu)

pu	32^3*	64^3*	256^3**
1	1.000	1.000	1.000
2	1.955	2.108	-
4	3.571	4.499	-
8	5.680	8.326	4.053
16	9.941	15.482	-

** : Cubic Driven Cavity (2nd Order) with MPI Message Passing Library*

*** : 3D Homogeneous Isotropic Turbulence (10th Order) with MPI Message Passing Library*

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Lattice Boltzmann Method

Lattice Boltzmann Equation

$$f_{\sigma i}(\mathbf{x}+\mathbf{e}_{\sigma i}, t+1) - f_{\sigma i}(\mathbf{x}, t) = \Omega_{\sigma i}$$

$f_{\sigma i}$: Single-Particle Distribution Function
$\Omega_{\sigma i}$: Collision Operator
$\mathbf{e}_{\sigma i}$: Velocity

Single Time Relaxation Approximation

Lattice Boltzmann BGK Equation

$$f_{\sigma i}(\mathbf{x}+\mathbf{e}_{\sigma i}, t+1) - f_{\sigma i}(\mathbf{x}, t) = -\frac{1}{\tau}\left[f_{\sigma i}(\mathbf{x}, t) - f_{\sigma i}^{(0)}(\mathbf{x}, t)\right]$$

$f_{\sigma i}^{(0)}$: Equilibrium Distribution Function
τ : Single Relaxation Time (=(6ν+1)/2)

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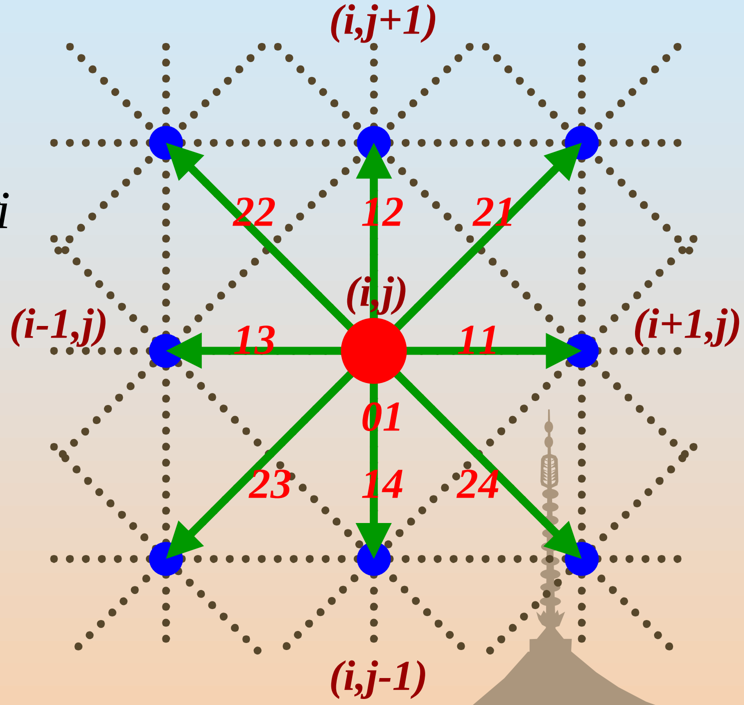
Lattice Boltzmann Method

Physical Quantities (ρ,u)

$$\rho = \sum_{\sigma}\sum_{i} f_{\sigma i}\,, \quad \rho\mathbf{u} = \sum_{\sigma}\sum_{i} f_{\sigma i}\mathbf{e}_{\sigma i}$$

In the case of square lattice model

σ=0,1,2 , i=1,2,3,4



Square Lattice Model

Equilibrium Distribution

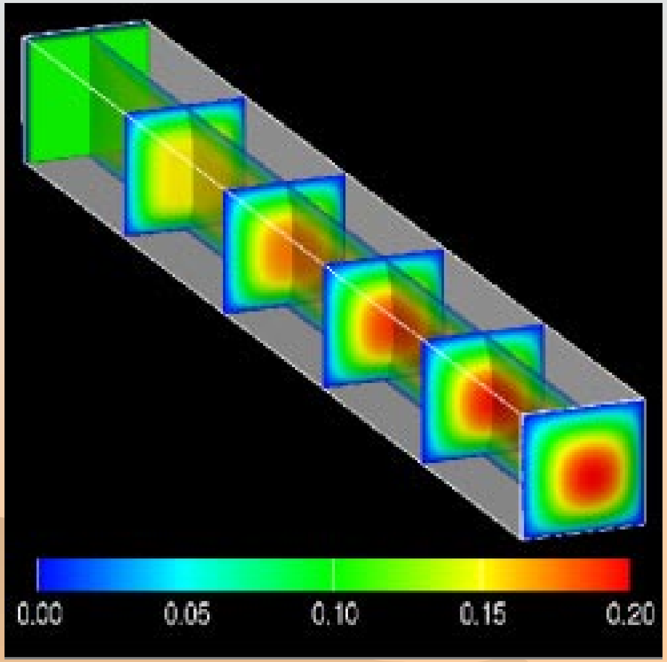
$$f_{01}^{(0)} = \rho\alpha - 3\rho\mathbf{u}^2/2$$

$$f_{1i}^{(0)} = \rho\beta + \rho(e_{1i}\cdot\mathbf{u})/3 + \rho(e_{1i}\cdot\mathbf{u})^2/2 - \rho\mathbf{u}^2/6$$

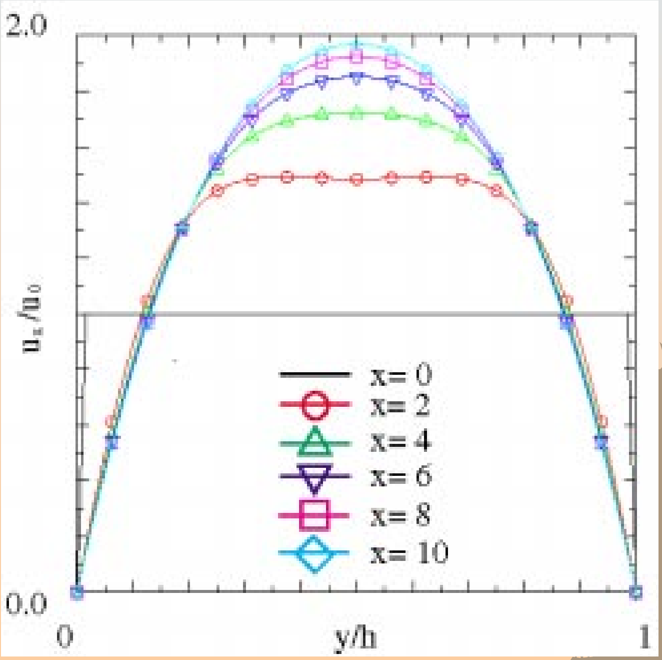
$$f_{2i}^{(0)} = \rho(1-\alpha-4\beta)/4 + \rho(e_{2i}\cdot\mathbf{u})/12 + \rho(e_{2i}\cdot\mathbf{u})^2/8 - \rho\mathbf{u}^2/24$$

DNS of Flows in Square Duct Using Lattice Boltzmann Method

Computational Conditions: 641x65x65 grid points
Re=200



Streamwise Velocity Distributions



Streamwise Velocity Profiles on the Center Plane

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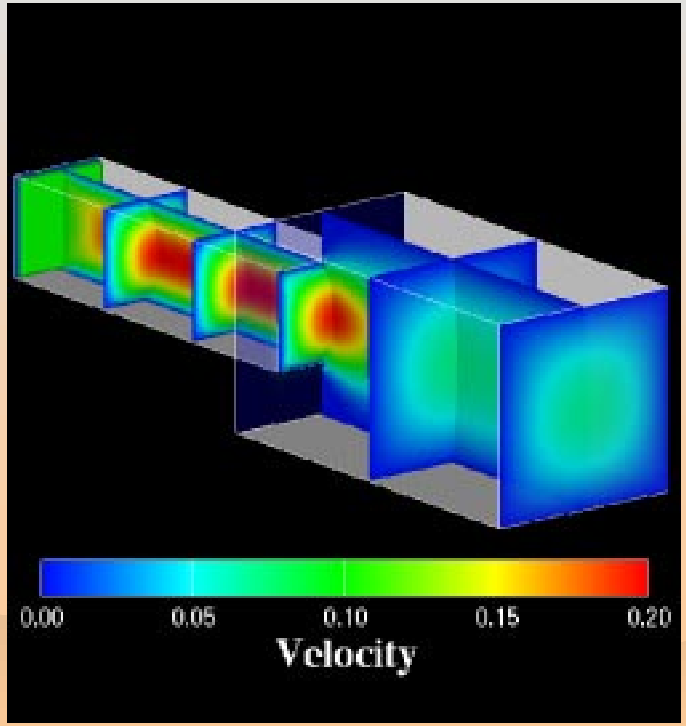
DNS of Flows in Square Duct with Sudden Expansion Using Lattice Boltzmann Method

Computational Conditions: Expansion Ratio 1:4
Re=10
128x33x33 (upstream)
129x65x65 (downstream)



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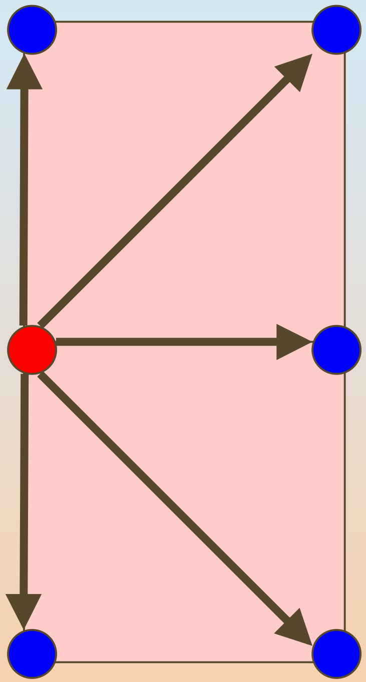
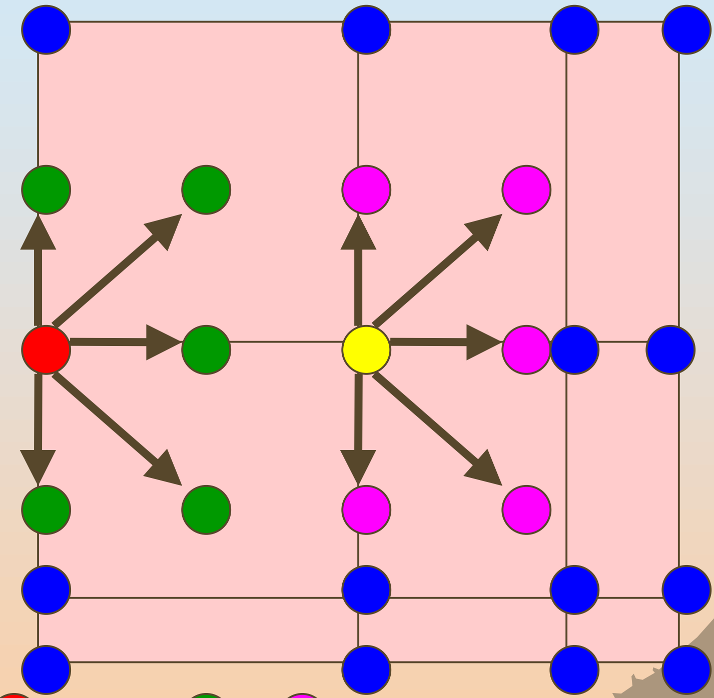
Lattice Boltzmann Method on Non-uniform Lattice



: n

: n+1

Usual Lattice Boltzmann



: n , : n+1

: n+1 on grid point (target)

By using interpolation and

Lattice Boltzmann on Non-uniform Lattice

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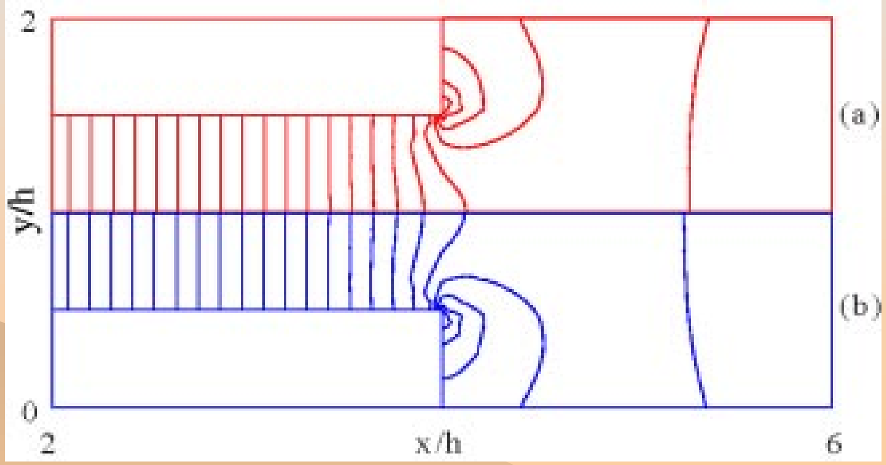
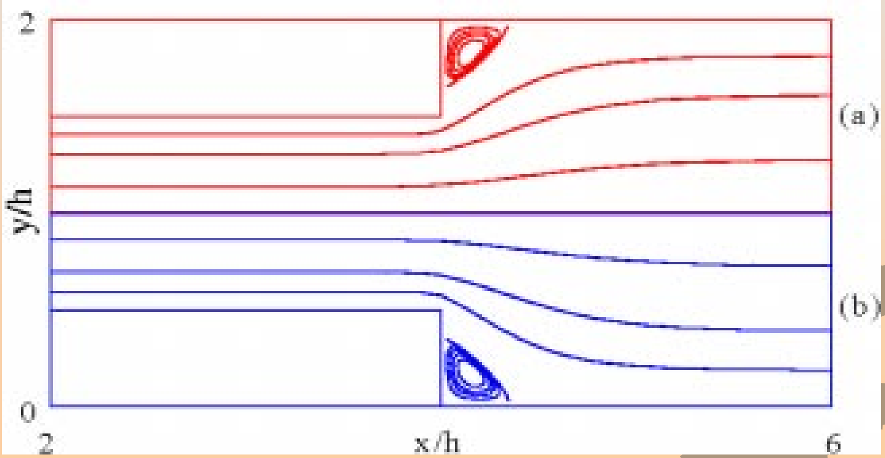
Lattice Boltzmann Method on Non-uniform Lattice

Validation of Non-uniform Lattice Approach

DNS of Flows in Channel with Sudden Expansion

Non-uniform Lattice (CPU Time Ratio 0.19)
Uniform Lattice (CPU Time Ratio 1.00)





Pressure Distributions

Stream Lines

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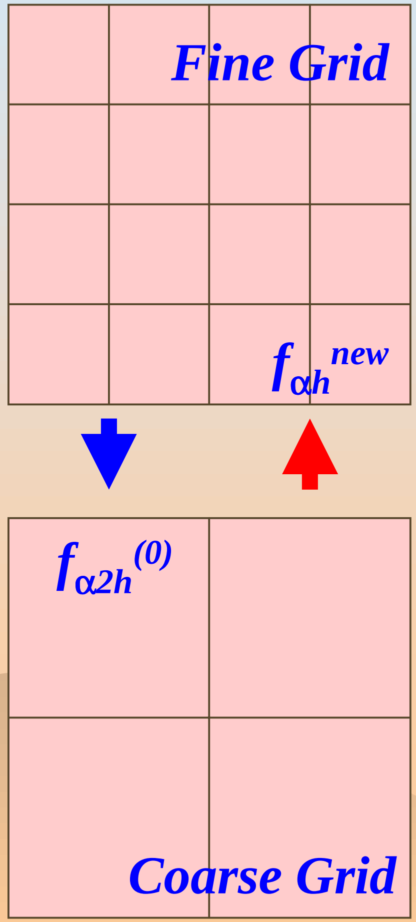
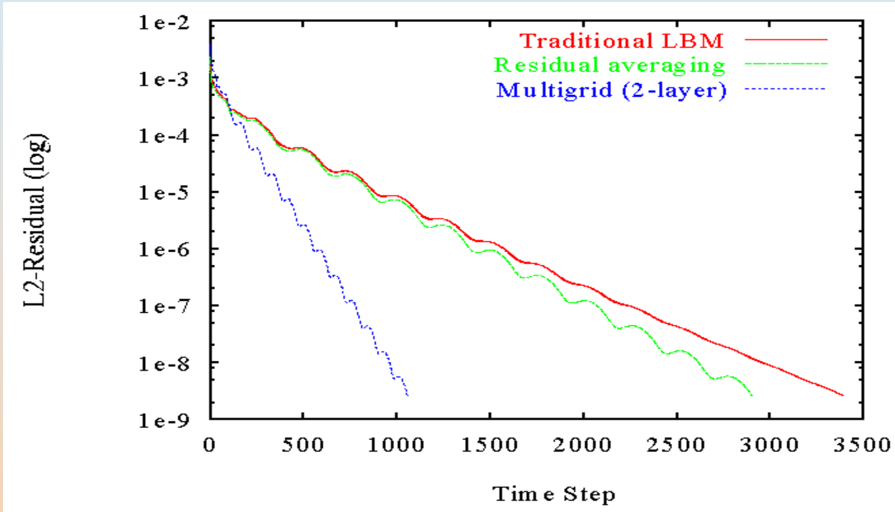
Lattice Boltzmann Method with Acceleration of Convergence

Multigrid Technique





Convergence History

Computational Time

LBM	*65x33*	*129x65*	*257x129*
Unigrid	*57.5 (1.00)*	*733.2 (1.00)*	*10564 (1.00)*
Multigrid	*24.7 (0.43)*	*436.4 (0.60)*	*5940 (0.56)*

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Parallelization

Lattice Boltzmann Method

3D Homogeneous Isotropic Turbulence

Speedup Ratio : T(1)/T(pu)

pu	32^3*	64^3*
1	1.000	1.000
2	1.754	1.851
4	2.984	3.323
8	4.505	5.460
16	5.622	8.162

* : MPI message passing library

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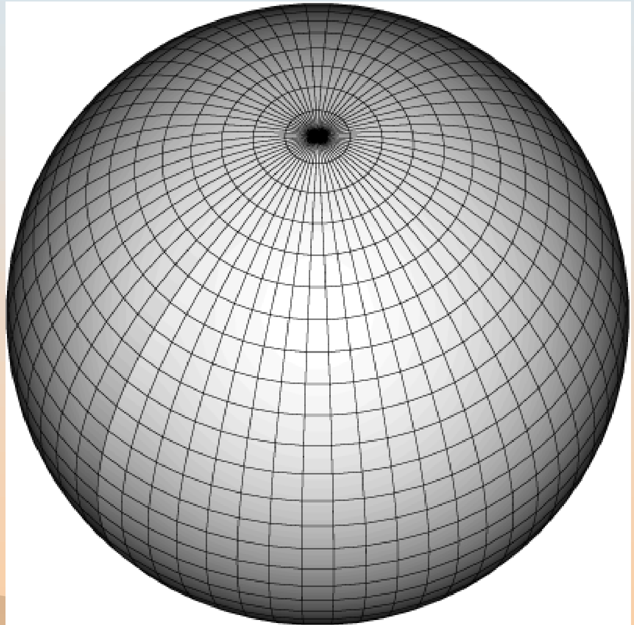
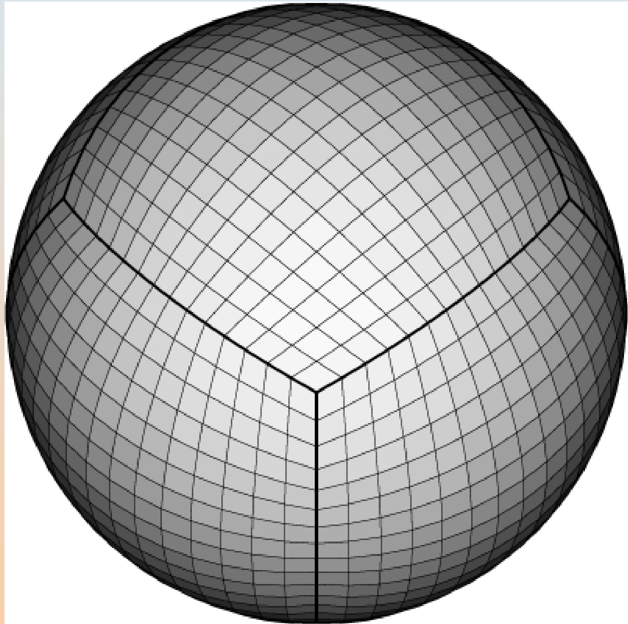
Cubed Sphere Coordinate System



Spherical Polar Coordinates



Cubed Sphere Coordinates

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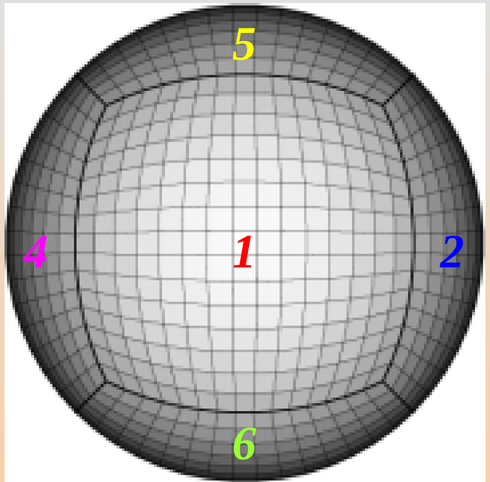
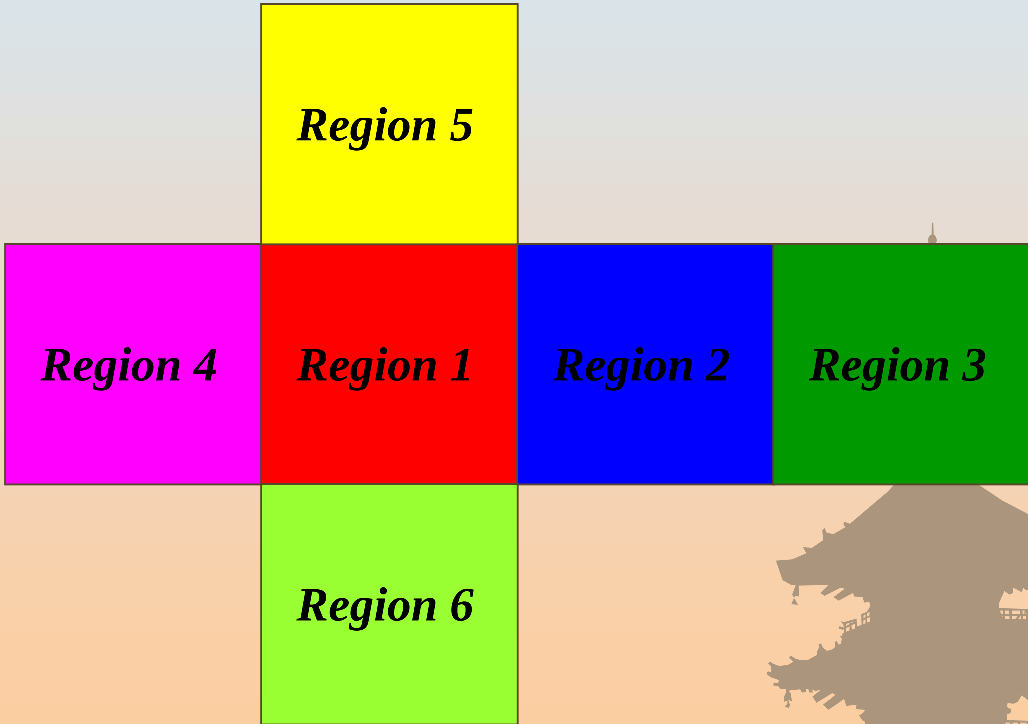
Cubed Sphere Coordinate System

Transformation Map





Physical Plane

Computational Plane

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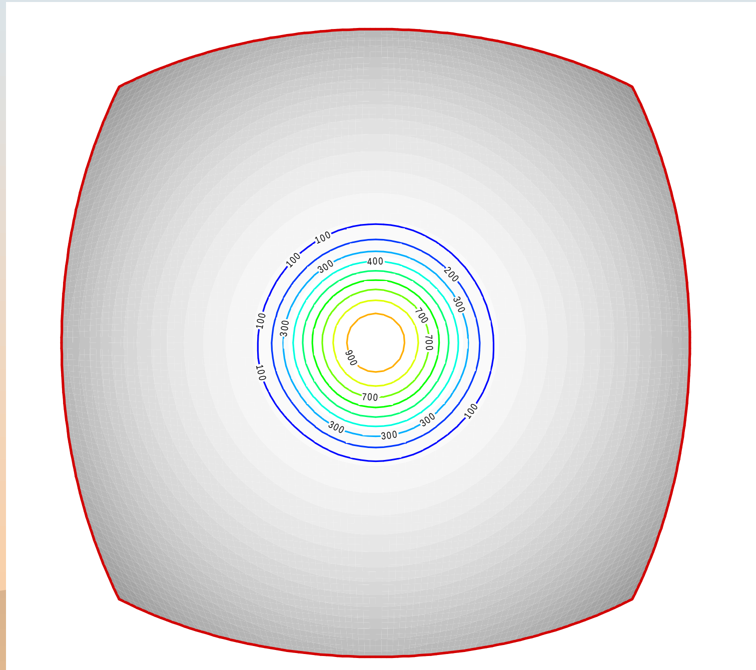
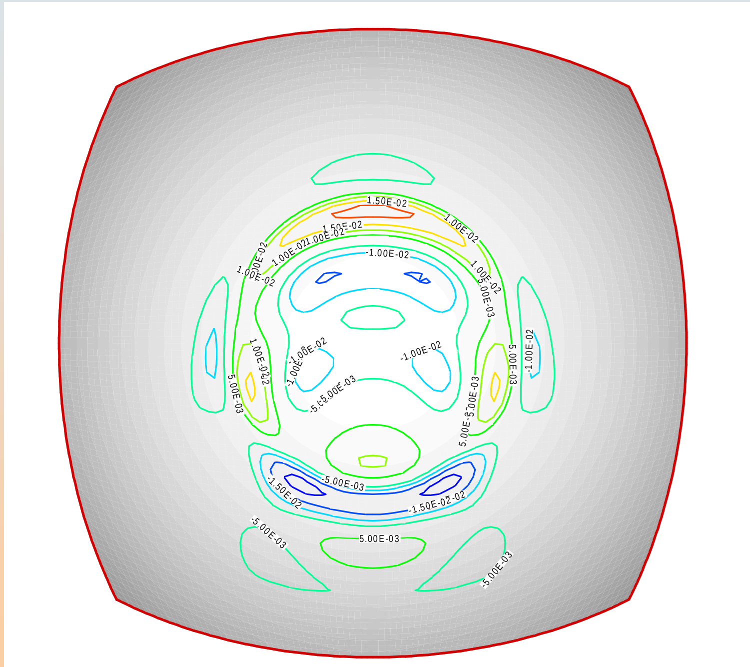
DNS of Flows on a Sphere Using Cubed Sphere Coordinates

Advection over Pole After 5 Full Rotations (Test Case : 1)



Hight



Error

4th Order Method of Lines (91^2x6 grid points)

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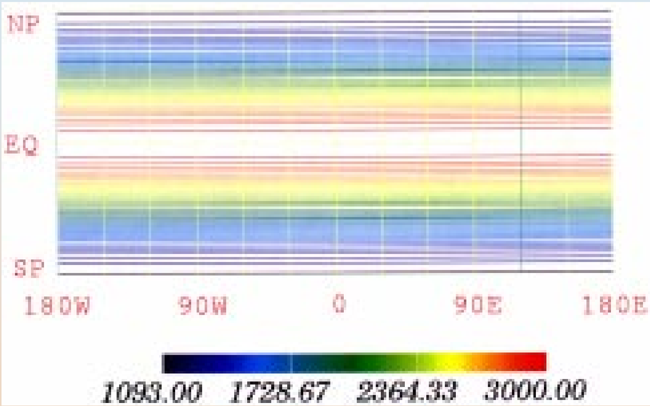
DNS of Flows on a Sphere Using Cubed Sphere Coordinates

Global Steady State Nonlinear Zonal Geostrophic Flow *(Test Case : 2)*

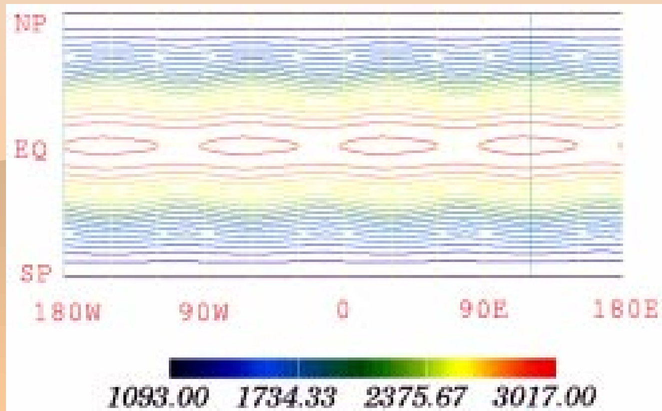


Analytic Hight

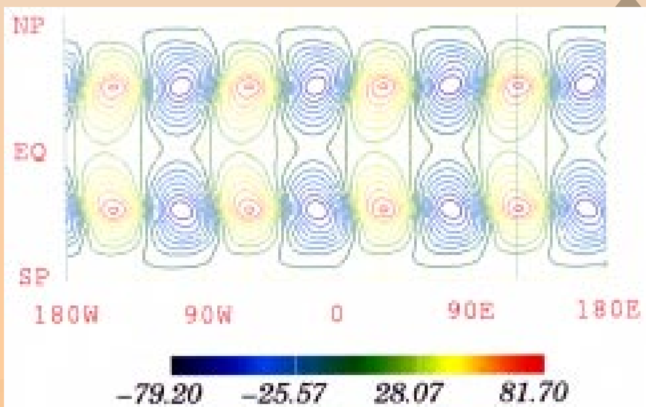
Shallow Water Equations

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} = -f\hat{\mathbf{k}}\times\mathbf{v} - g\nabla h$$

$$\frac{\partial h^*}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} + h^*\nabla\cdot\mathbf{v} = 0$$



Hight After 5 Days



Error

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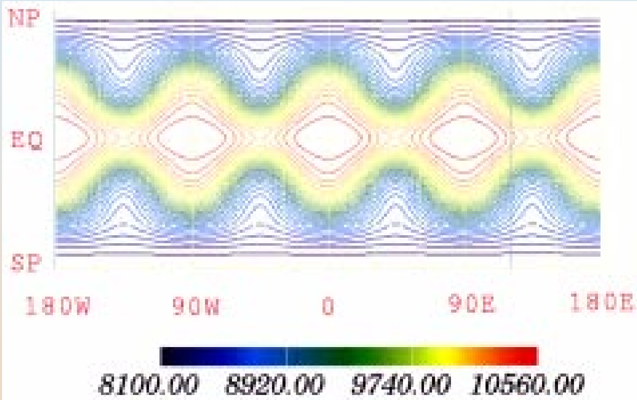
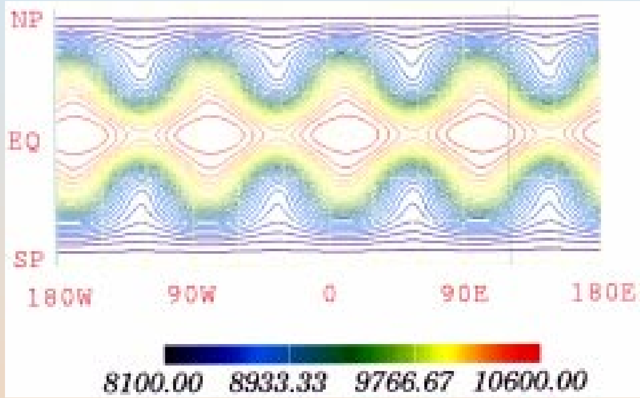
DNS of Flows on a Sphere Using Cubed Sphere Coordinates

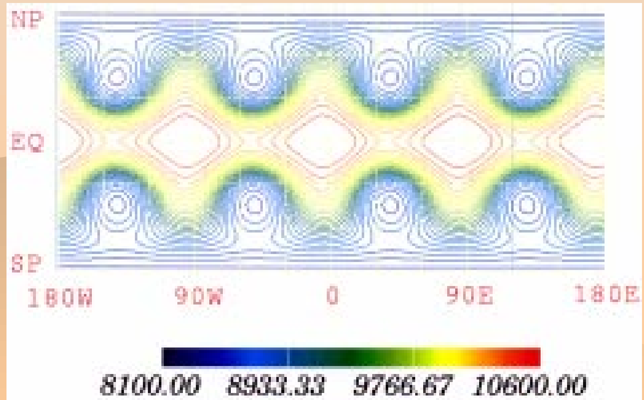
Rossby-Haurwitz Wave (Test Case : 6)



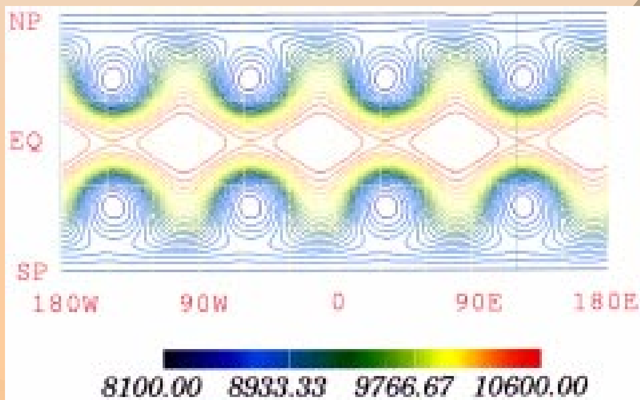
Day 0



Day 1



Day 7



Day 14

Hight Profiles

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Parallelization

Cubed Sphere Coordinates

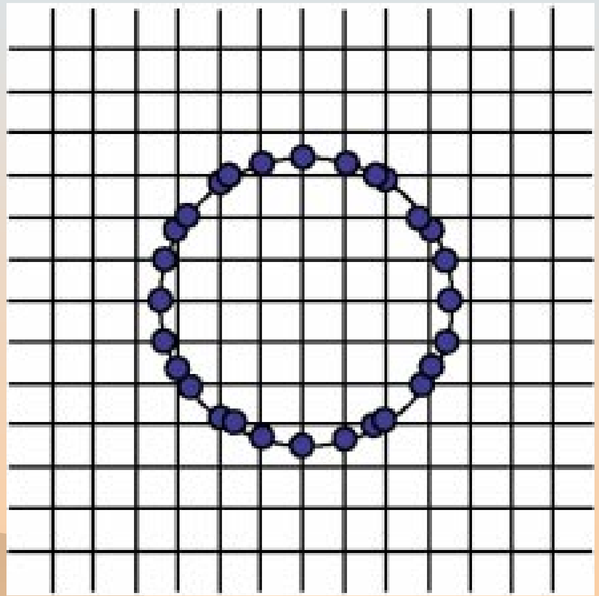
Advection over Pole After 5 Full Rotations

Speedup Ratio : T(1)/T(pu)

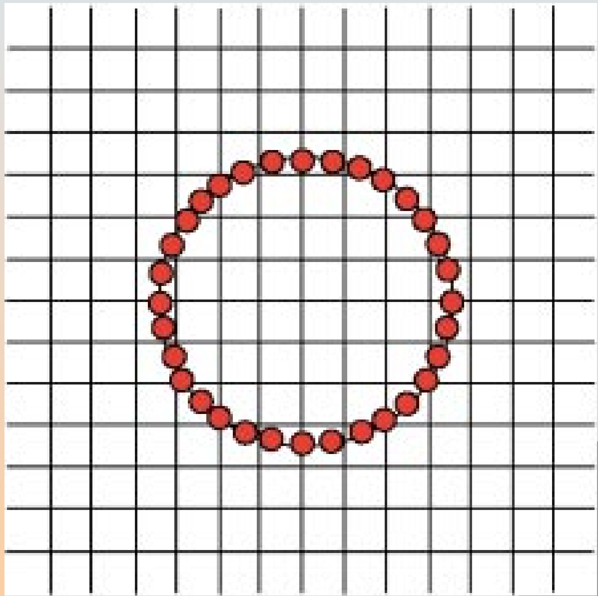
pu	91^2 *	181^2 *	901^2 *
1	1.000	1.000	1.000
6	7.815	8.253	5.943

** : MPI message passing library*

Cartesian Grid Approach with Virtual Boundary Method



Usual Cartesian Grid Approach



Cartesian Grid Approach with Virtual Boundary Method

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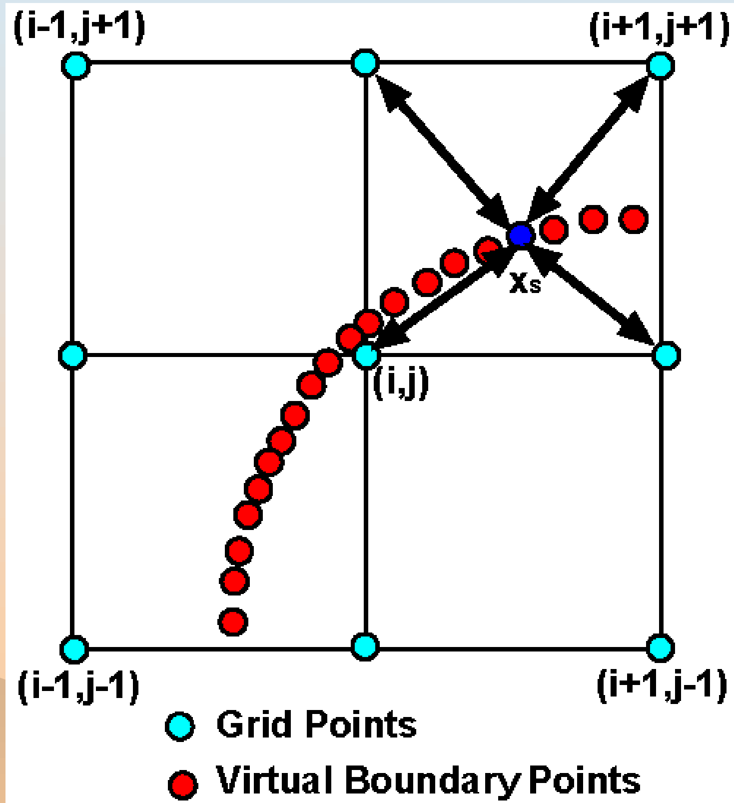
Cartesian Grid Approach with Virtual Boundary Method



Velocity on Virtual Boundary Point: $U_i(x_s)$

$$U_i(\mathbf{x}_s) = \sum_{\mathbf{x}_k}^{\mathbf{x}_k+1} Q_{\mathbf{x}_k}(\mathbf{x}_s)\, u_i(\mathbf{x}_k)$$

Additional Forcing Term: $G_i(x_s,t)$

$$G_i(\mathbf{x}_s,t) = \alpha\int_0^t U_i(\mathbf{x}_s,t)\,dt + \beta U_i(\mathbf{x}_s,t)$$

Modified Navier-Stokes Equations:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_i^2} + G_i$$

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DNS of Flows Around a Sphere

Computational Conditions
Re=500 , Virtual Boundary Points: 153600
Total Cartesian Grid Points: 973744

Iso-Surface of $\nabla^2 p$

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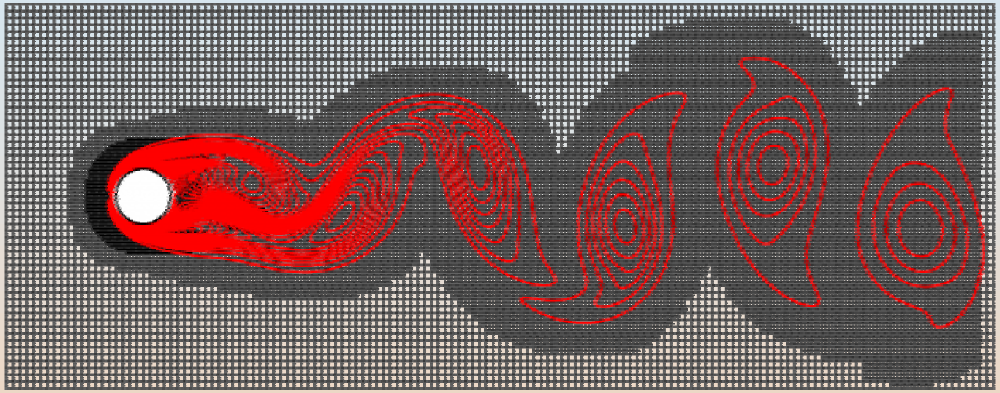
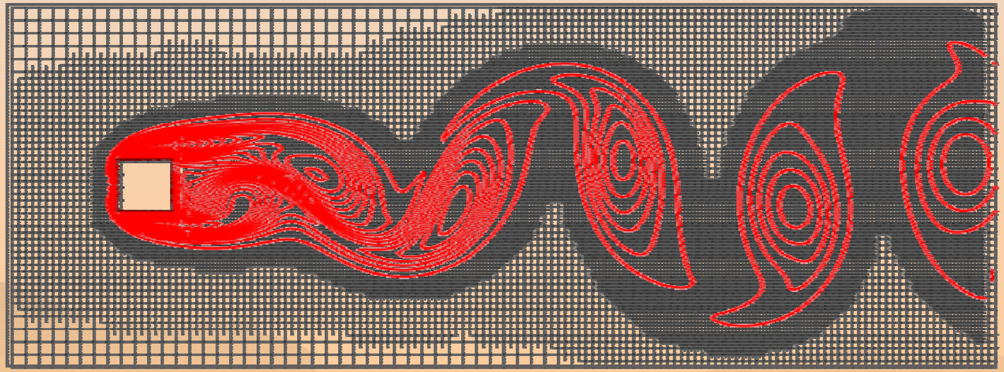
Cartesian Grid Approach with Adaptive Grid Refinement



Re = 100 (with Virtual Boundary Method)



Re = 100 (without Virtual Boundary Method)

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研究達成状況

●高次精度線の方法
- 3次元一様等方性乱流　○
- 並列化　△

●格子ボルツマン法
- 3次元正方直管内流れ　○
- 3次元急拡大管内流れ　○
- 並列化　△

●立方化球座標系
- 球面上移流方程式　○
- 球面上浅水波方程式　○
- 並列化　○

●仮想境界デカルト格子法
- 球周りの流れ　○
- 解適応デカルト格子　○

JSPS
Research for the Future Program

今後の研究計画

●平成12年度

- *並列化効率の向上*
  (高次精度線の方法、格子ボルツマン法)
- *解適応格子アルゴリズムとのカップリング*
- *コリオリ力を考慮した**Navier-Stokes***
  シミュレーションコードの開発
- *基礎的環境シミュレーションの実施*

●平成13年度

- *高精度大規模数値シミュレーションの実施*
  (高次精度線の方法、格子ボルツマン法)
- *シミュレーション結果のデータベース化*
- *名古屋大学グループと共同で地球規模流動現象*
  解明のための計算科学的手法の提示