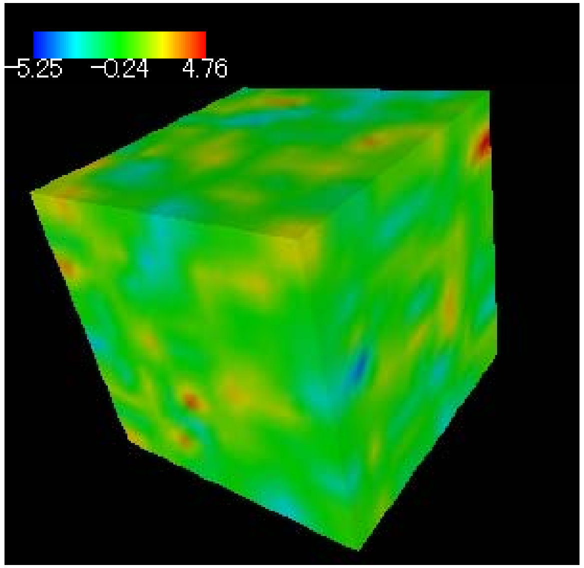
解析対象

- 透水係数が空間的に分布する三次元地下水流れ
  - ポアソン方程式
  - 透水係数は地質統計学的手法によって決定〔Deutsch & Journel, 1998〕
- 規則正しい立方体ボクセルメッシュを使用した有限体積法
  - 局所細分化を考慮
- 周期的な不均質性: 128^3

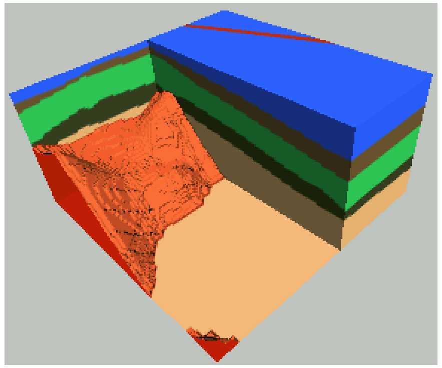
$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial\phi}{\partial z}\right)=q$$

$$\phi=0 @ x=x_{\max}$$

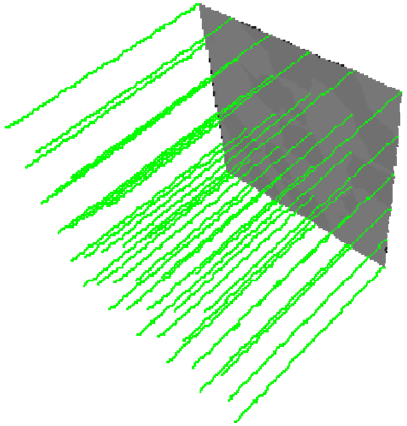


Groundwater Flow through Heterogeneous Porous Media

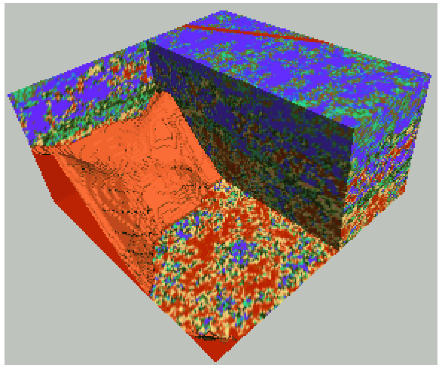
Homogeneous



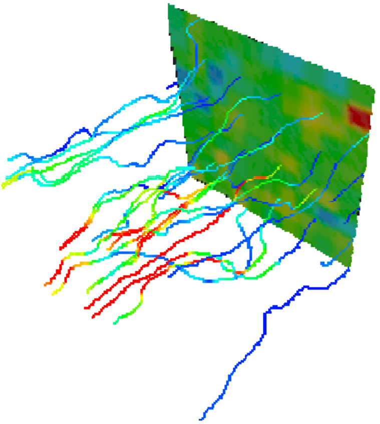
Uniform Flow Field



Heterogeneous

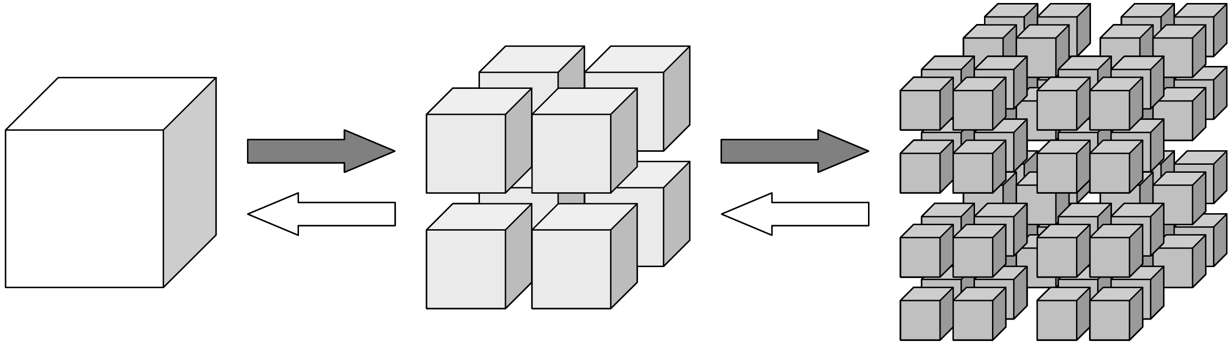


Random Flow Field



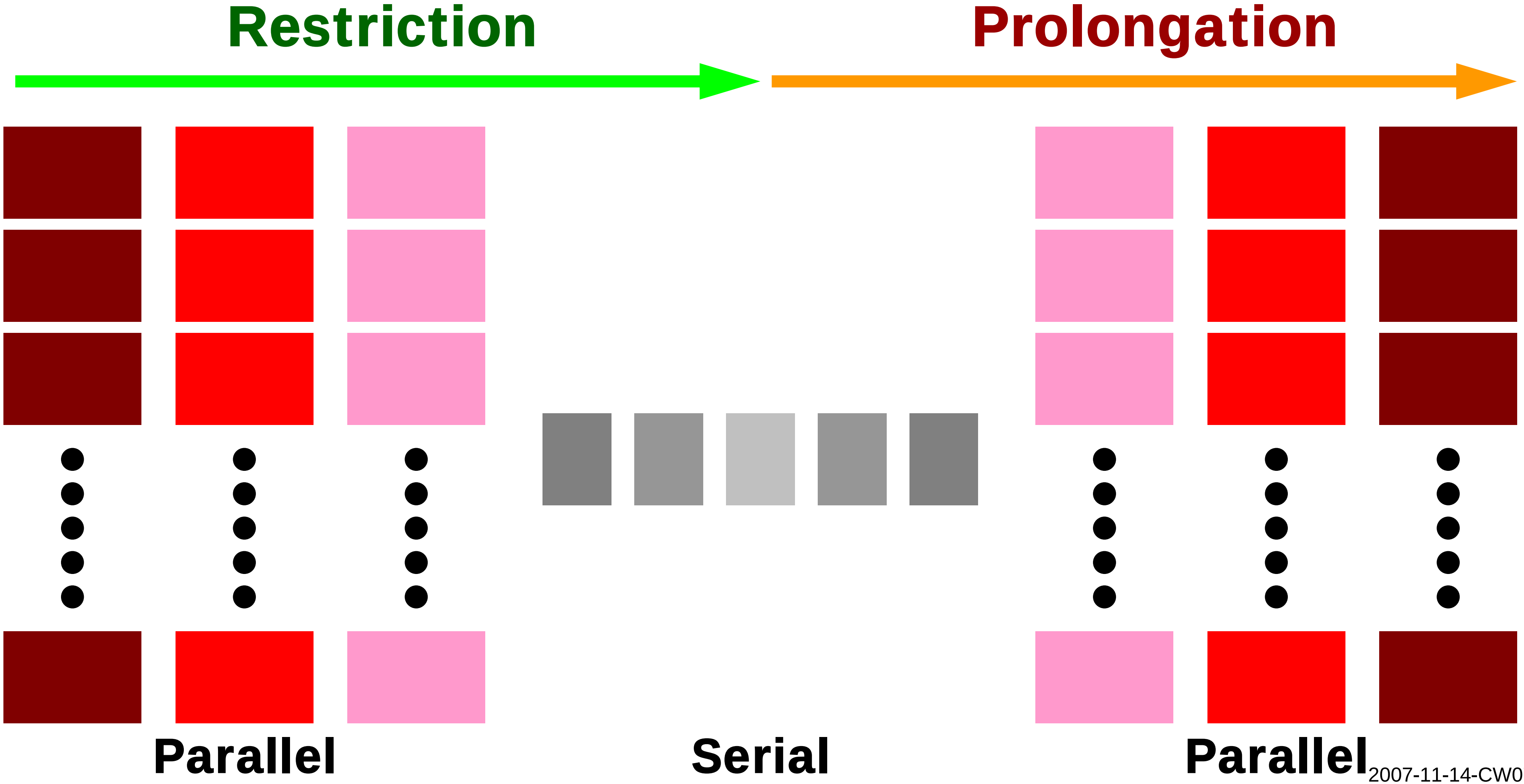
線形ソルバーの概要

- 前処理付きCG法
  - Multigrid 前処理
  - IC(0) for Smoothing Operator (Smoother)
  - Additive Schwartz Domain Decomposition
- 並列（幾何学的）多重格子法
  - 等方的な8分木
  - V-cycle
  - 領域分割型：Block-Jacobi局所前処理，階層型領域間通信
  - 最も粗い格子（格子数＝プロセッサ数）は1コアで実施



並列，シリアル計算の切り替え

粗いレベルではシリアル計算に切り替える
本プログラムでは最も粗いレベルのみシリアル計算



IC(0) as smoother of Multigrid

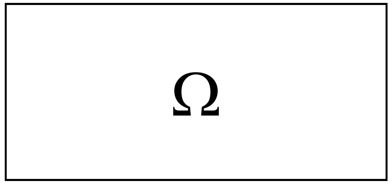
- IC(0) is generally more robust than GS.
- IC(0) smoother with Additive Schwartz Domain Decomposition (ASDD) provides robust convergence and scalable performance of parallel computation, even for ill-conditioned problems〔KN 2002〕.

Overlapped Additive Schwartz Domain Decomposition Method

for Stabilizing Localized Preconditioning

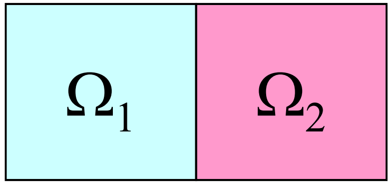
Global Operation

$$Mz = r$$



Local Operation

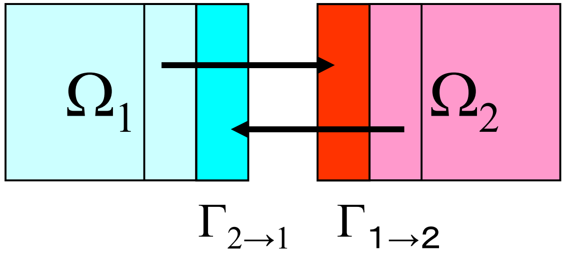
$$M_{\Omega_1} z_{\Omega_1}^{n} = r_{\Omega_1}, \quad M_{\Omega_2} z_{\Omega_2}^{n} = r_{\Omega_2}$$



Global Nesting Correction

$$z_{\Omega_1}^{n} \leftarrow z_{\Omega_1}^{n-1} + M_{\Omega_1}^{-1}\left(r_{\Omega_1} - M_{\Omega_1} z_{\Omega_1}^{n-1} - M_{\Gamma_{2\to1}} z_{\Gamma_{2\to1}}^{n-1}\right)$$

$$z_{\Omega_2}^{n} \leftarrow z_{\Omega_2}^{n-1} + M_{\Omega_2}^{-1}\left(r_{\Omega_2} - M_{\Omega_2} z_{\Omega_2}^{n-1} - M_{\Gamma_{1\to2}} z_{\Gamma_{1\to2}}^{n-1}\right)$$



Hardware/Software

- T2K/Tokyo
  - up to 512 nodes (8,192 cores)
- Program
  - Hitachi FORTRAN90 + MPI
  - CRS matrix storage
  - CM-RCM Reordering for OpenMP

```
for (i=0; i<N; i++) {
  for (k=Index(i-1); k<Index(i); k++{
    Y[i]= Y[i] + A [k]*X[Item[k]];
  }
}
```

- $|Ax-b|/|b|=10^{-12}$ for Convergence
- 不均質性
  - 最大最小透水係数の比 $= 10^{10}$ (10^{-5}~10^{+5})
- Multigrid Cycles
  - 1 V-cycle/iteration
  - 2 smoothing iterations for restriction/prolongation at every level
  - 1 ASDD iteration cycle for each resrtiction/prolongation

Weak Scaling

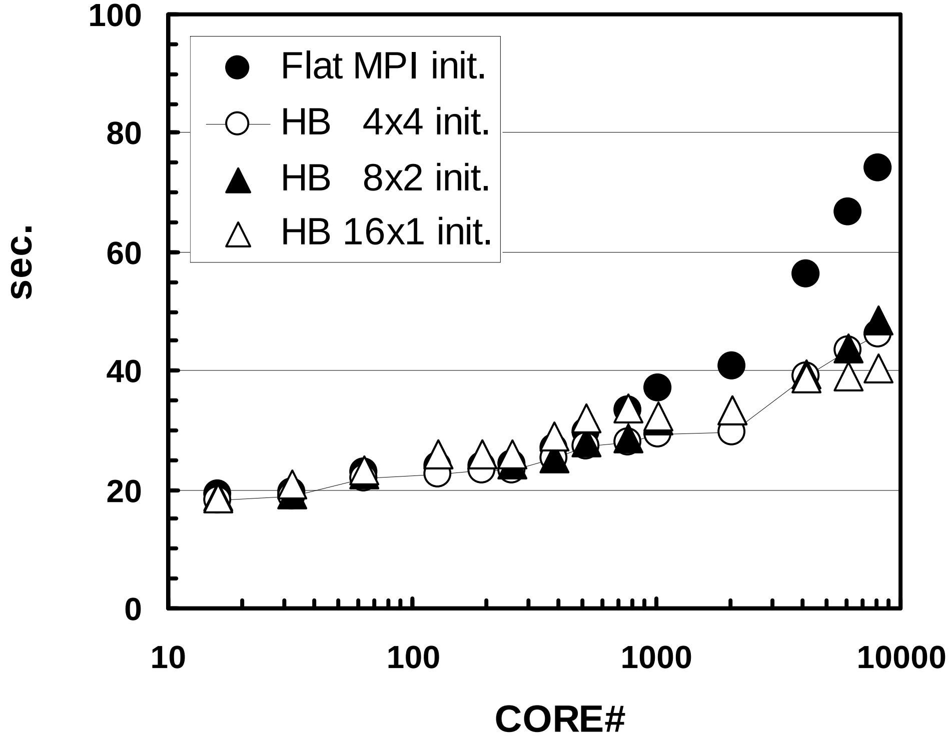
- コアあたりの問題規模を固定
  - Scalableであれば，コア数を増やして全体の問題規模が大きくなっても反復回数が変わらないため，計算時間は変わらないはず（実際はそううまく行かない）。
  - 全体の問題規模を固定するのがStrong Scaling

- Up to 8,192 cores (512 nodes)
  - 64^3 cells/core
  - 2,147,483,648 cells

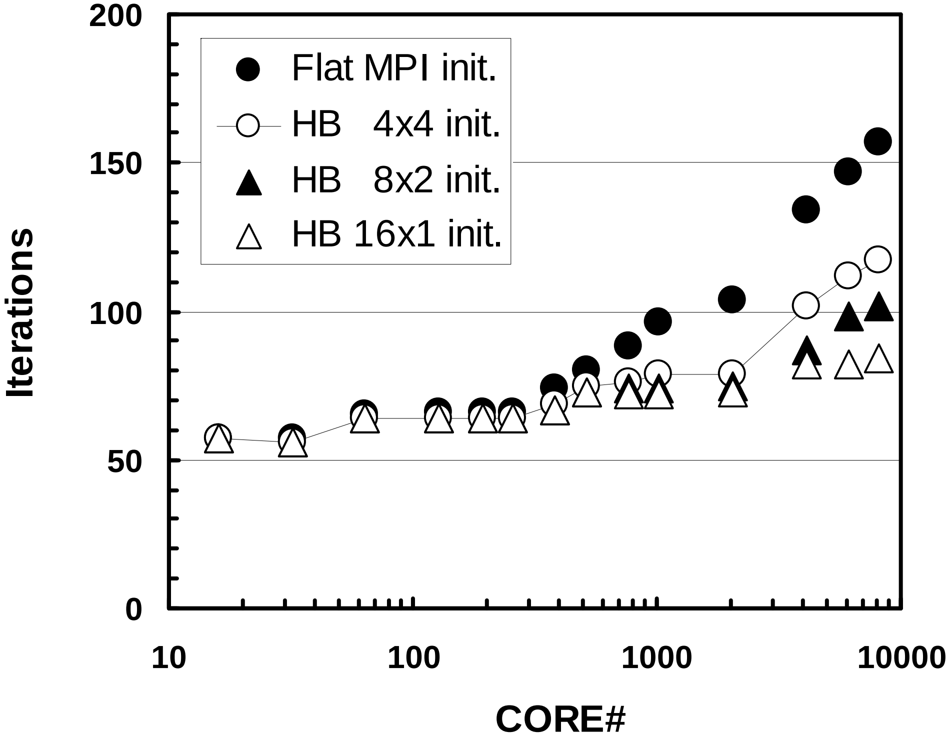
Weak Scaling

64^{3}cells/core, up to 8,192 cores (2.05 × 10^9 cells)

sec.

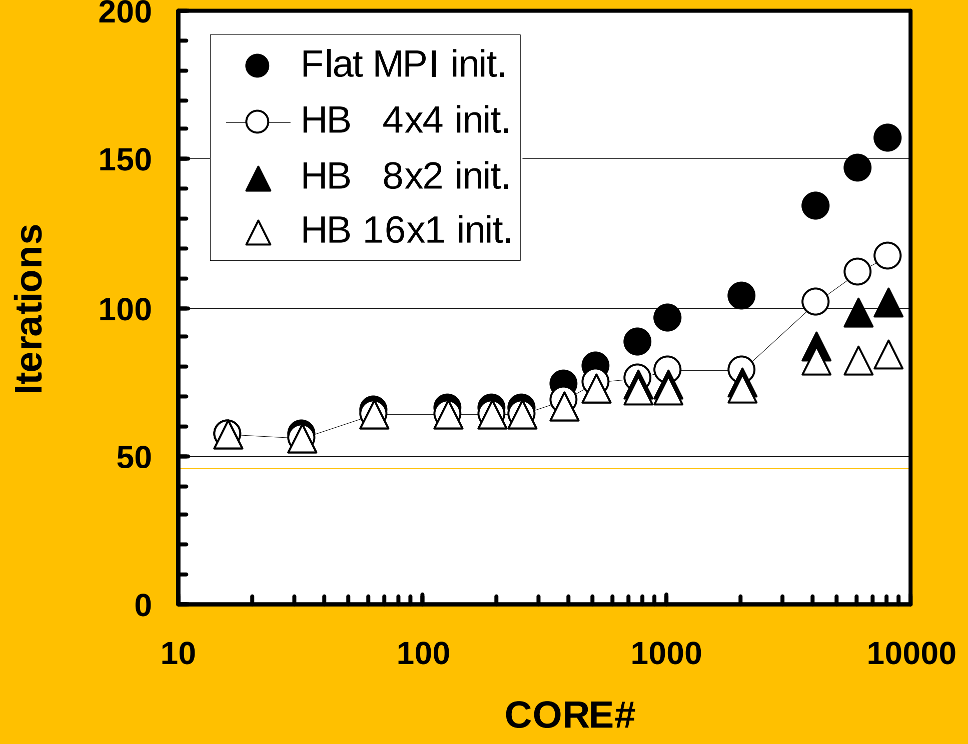


Iterations



Coarse Grid Solverの改良

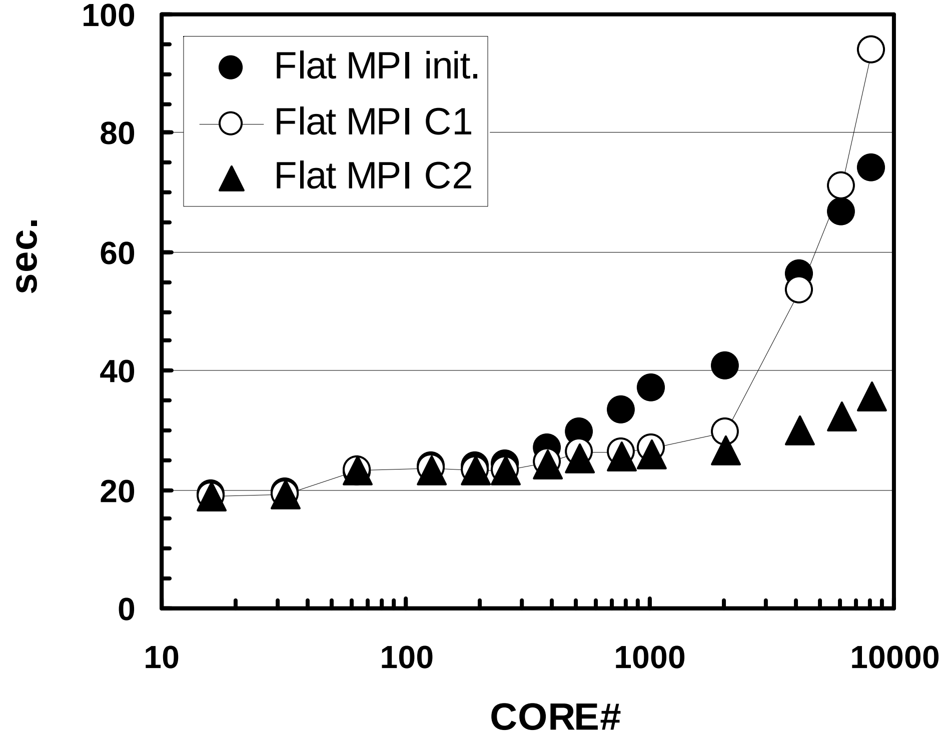
- 領域数が増えると反復回数が増加（特にFlat MPI）
- 最も粗い格子（Coarse Grid Solver）
  - 各領域1メッシュになった状態で1コアに集める
  - IC(0)スムージングを一回施す
- Coarse Grid Solver改良
  - IC(0)スムージングを収束（$\varepsilon=10^{-12}$）まで繰り返す：C1
  - マルチグリッド（V-cycle）を適用し，収束（$\varepsilon=10^{-12}$）まで繰り返す（8,192=32×16×16）：C2



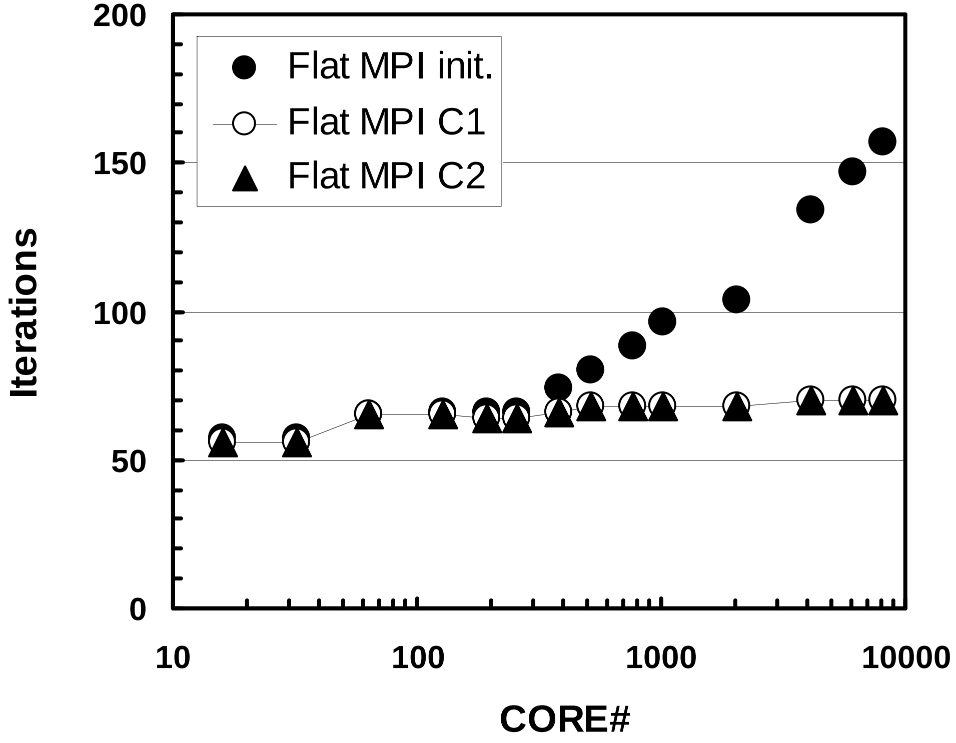
Weak Scaling: Flat MPI

64^3cells/core, up to 8,192 cores (2.05×10^9 cells)

sec.



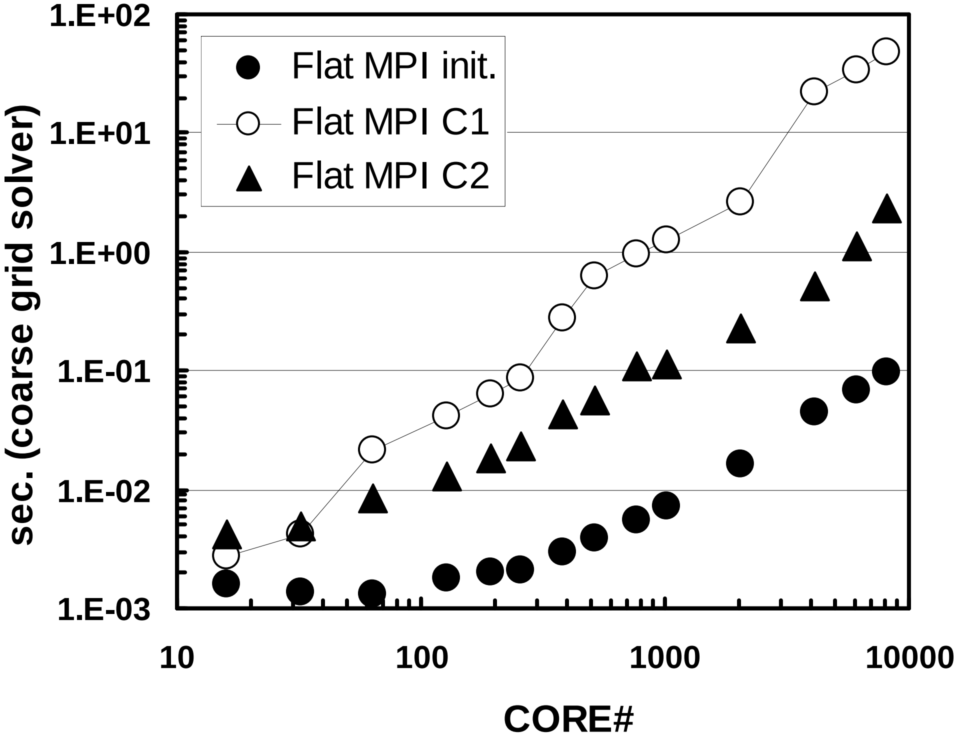
Iterations



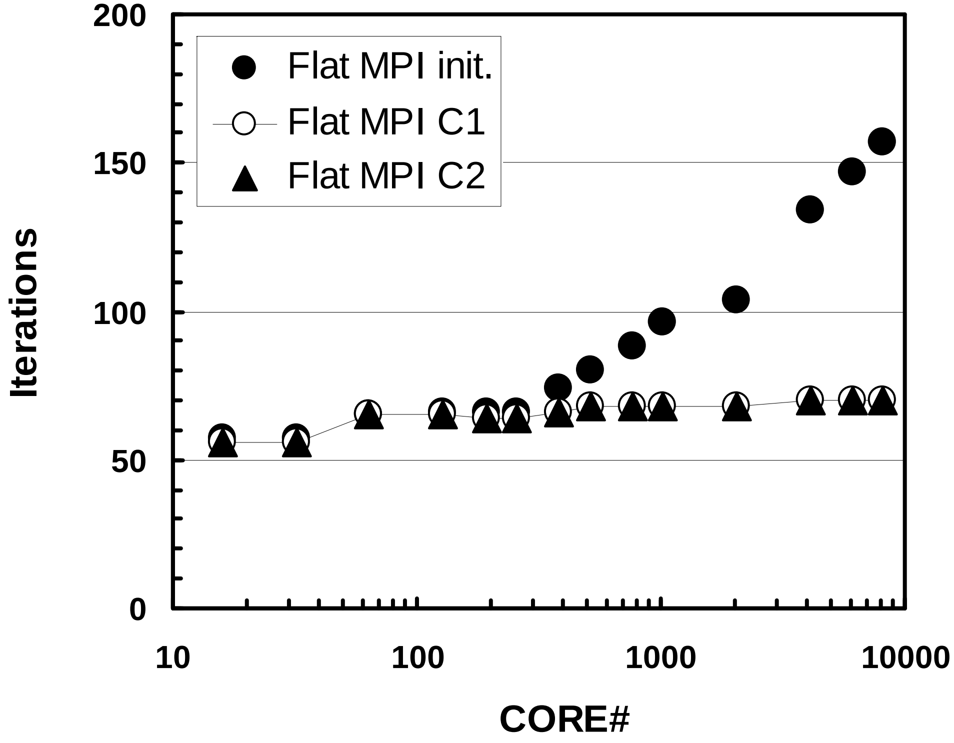
Weak Scaling: Flat MPI

64^3cells/core, up to 8,192 cores (2.05×10^9 cells)

Coarse Grid Solver



Iterations

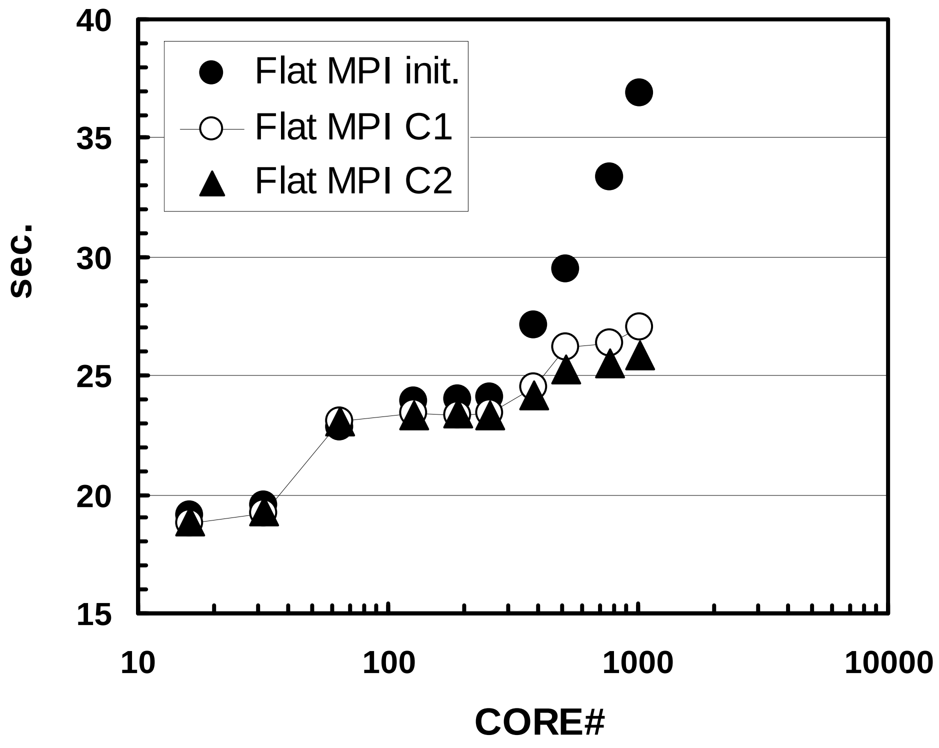


Weak Scaling: Flat MPI

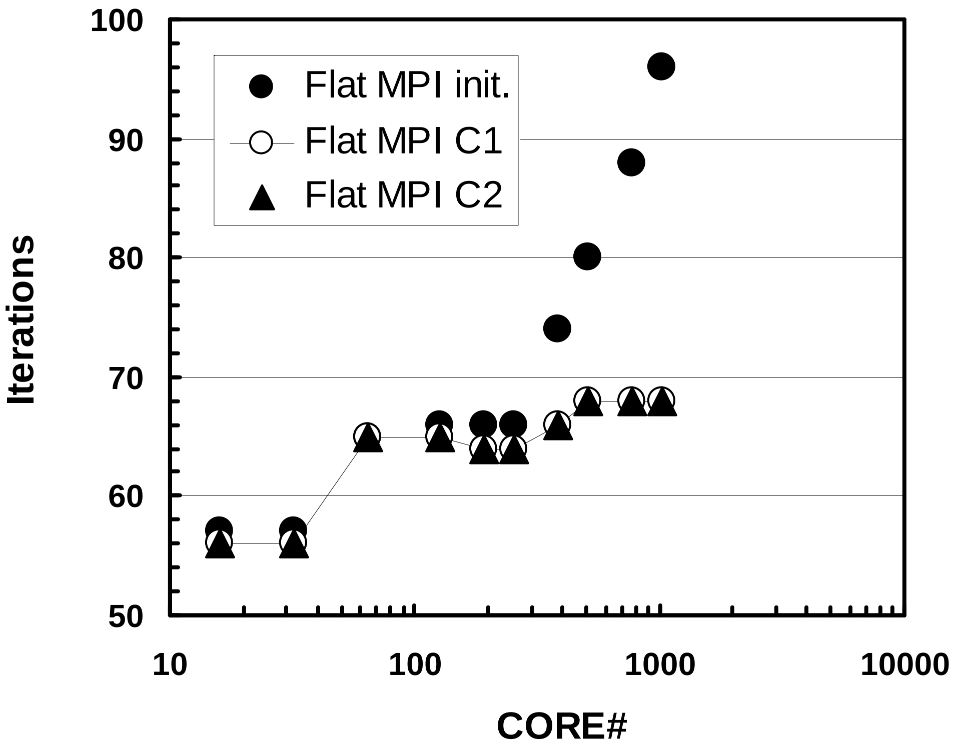
64^3cells/core, up to 8,192 cores (2.05×10^9 cells)

256コア程度までは変わらない

sec.



Iterations

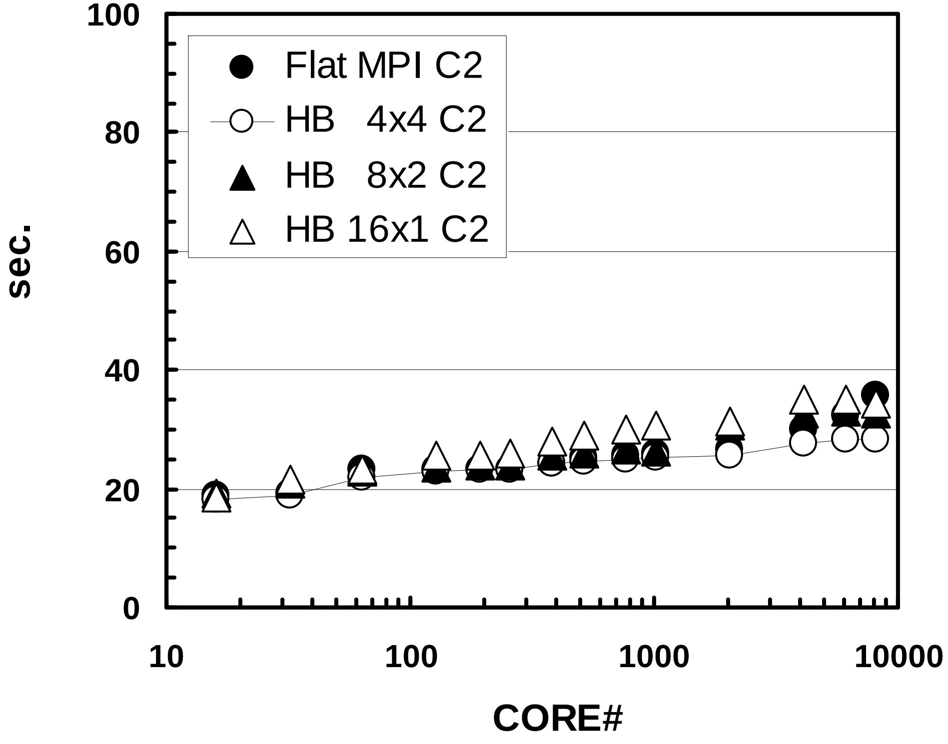


Weak Scaling：改良後　ほぼScalable

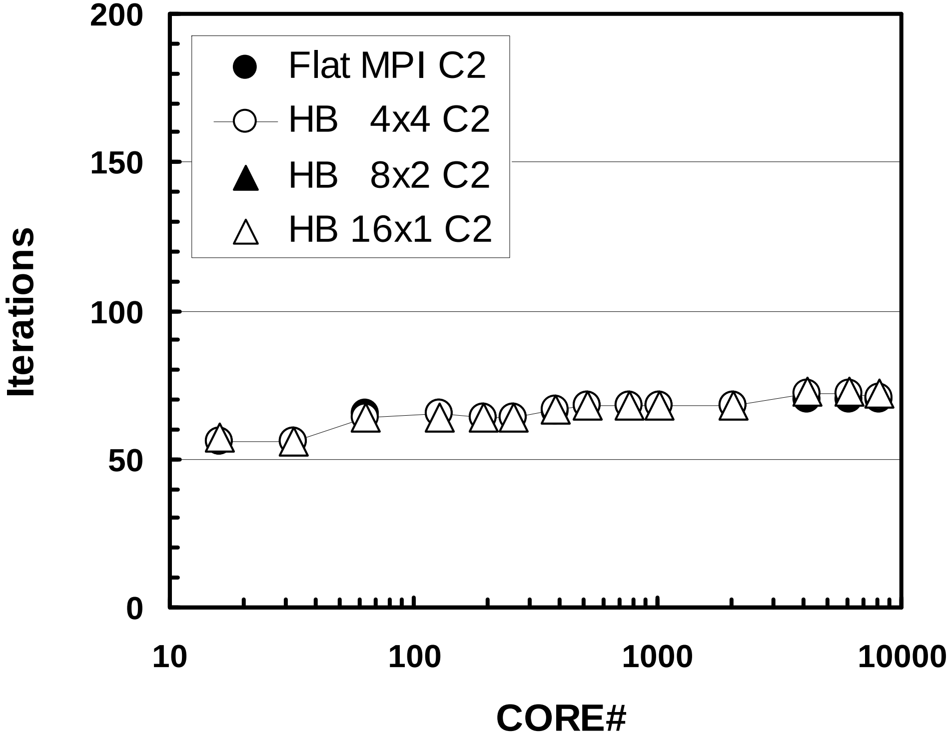
64^3cells/core, up to 8,192 cores (2.05×10^9 cells)

at 8,192 cores: Flat MPI(35.7sec), HB 4x4(28.4), 8x2(32.8), 16x1(34.4)

sec.

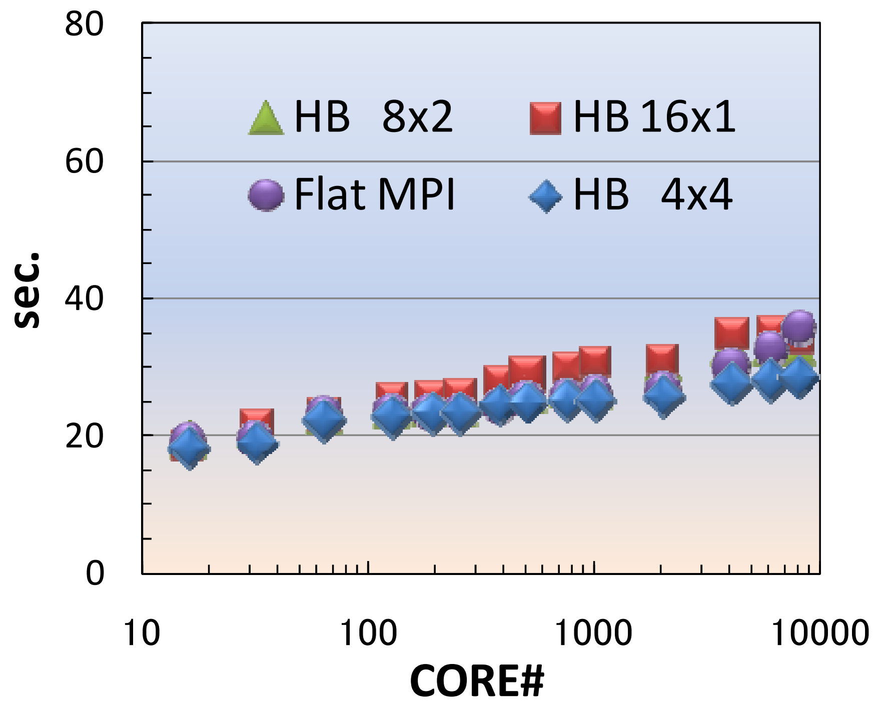


Iterations

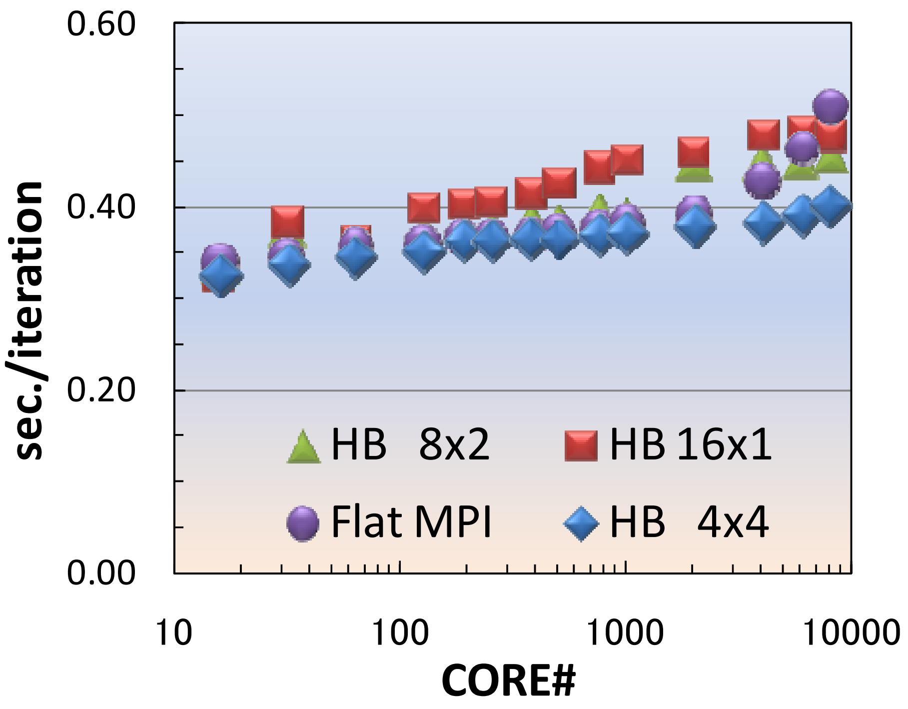


でもよく見るとScalableではない
通信のオーバーヘッド等

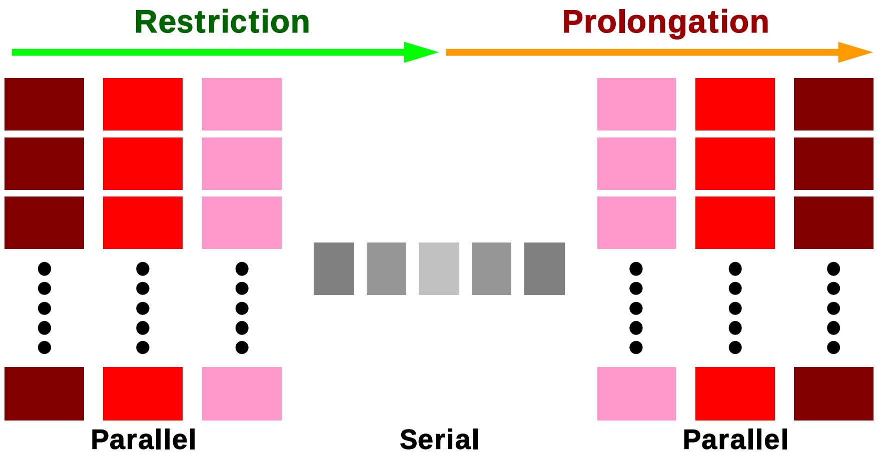
sec.



Iterations



多重格子法(Multigrid)の課題



- 悪条件問題への対応
  - Smoother
- 不規則形状への対応
  - 代数的マルチグリッド
- 超並列計算
  - オーバーヘッド削減
  - 粗い格子での処理
  - 大規模になって初めて見えてくることはある