Convergence Acceleration of the PinT Integration of Advection Equation using Accurate Phase Calculation Method

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Convergence Acceleration of the PinT Integration of Advection Equation using Accurate Phase Calculation Method

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to be tackled by using Post ‘K’ Computer.

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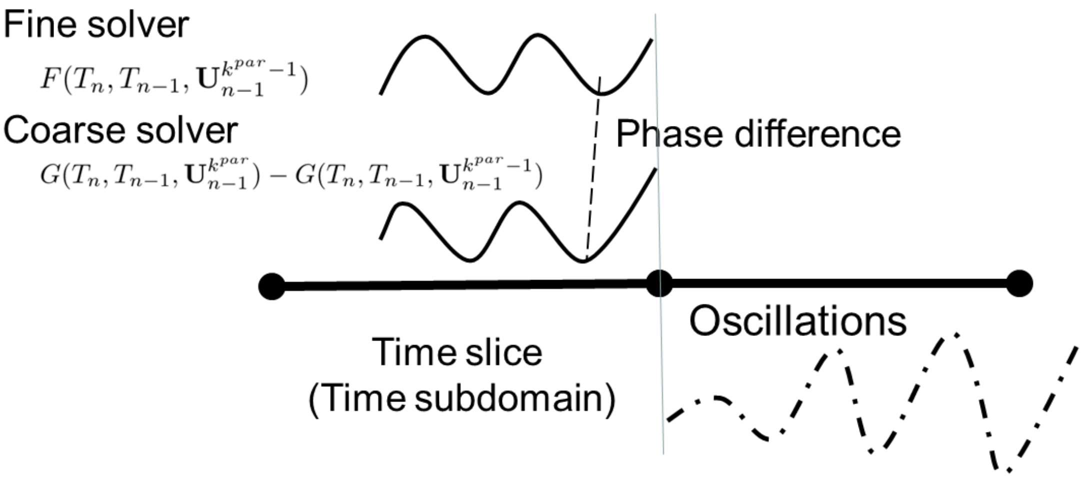
Issue and Challenge

■ Issue of the parareal method for hyperbolic PDEs:



*M. Gander and M. Petcu, Analysis of a Krylov subspace enhanced parareal algorithm for linear problems, ESAIM Proc, 25, (2008), 114-129.

Hyperbolic PDEs: Waves →
There is Phase Difference between fine and coarse solver's result →
Oscillations → damages the convergence of the parareal method

■ Challenge:

- **Improvement of the convergence**

→ We must reduce the phase difference between fine and coarse solvers (≒ phase error).

(We just focus on the convergence.)

How do we perform reducing phase error?

Expected methods to reduce phase error in coarse solver with low cost

		To reduce the cost		
		Coarsening		Coarsening time step width $\delta T >> \delta t$
		Space	Time integrator	
To increase the phase accuracy	Using fine δt as δT coarse solver time step width	Using coarse space modes → High accurate convergence is not available by lack of high order space modes.	Using low cost time integrator → Available for only the case that fine solver cost is very high.	
	Using a high accuracy phase calculation method			Using high order time integrator→ Not enough CIP scheme + STRS scheme

Ex: CAAP method

For advection term calculation

We focus on mainly CIP scheme in this presentation.

Method overview

Methods overview of advection term calculation

Conventional main method

$$\partial_t \phi + c\partial_x \phi = 0$$

Stabilization:
numerical damping
Accuracy:
Space and time
higher order terms

Methods that are tried in this study

(1) CIP scheme: advecting the phase information by the gradient of value Φ.

$$\partial_t \phi + c\partial_x \phi = 0$$

$$\partial_t g + c\partial_x g = 0$$

$$g = \partial_x \phi$$

(3)Hybrid STRS-CIP

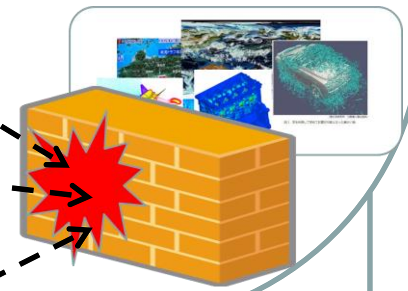
$$\partial_{t'} \phi + c\partial_{x'} \phi = 0$$

not enough

not yet success

There is a limit in the use.

Main issue : Gap of phase accuracy between fine and coarse solver



(2) STRS scheme: achieving the stabilization and error elimination using “space and time reversal symmetry “ .

We focus on the CIP in this study.

What is CIP(constrained Interpolation Profile) scheme?

・proposed by T. Yabe eta(1987)*

＊ H. Takewaki and T. Yabe, The cubic-interpolated pseudo particle (CIP) method: Application to nonlinear and multi-dimensional hyperbolic equations, J. Comput. Phys., 70 (1987), 353372.

・performs numerical advection process by the semi-Lagrange method using the cubic interpolation function of **both variable and its gradient**.

The CIP scheme gives the accurate phase.

Why ?

The method **using a space differential of the equation** gives generally **highly precise solutions even on coarse grids**.

- CIP3rd scheme:

(a) $\partial_t \phi + c\partial_x \phi = 0$

(b) $\partial_t g + c\partial_x g = 0$

$g = \partial_x \phi$

- Mixed form of FEM :Handle these equations as PDE

(Structure analysis)

(a) Equation of strain and displacement relation

(b) Equation of moment conservation

- FIC scheme

(Finite Increment Calculus)

(a) $r_s := \rho c u \frac{d\phi}{dx} - \frac{d}{dx}\left(k\frac{d\phi}{dx}\right) + s\phi - Q$

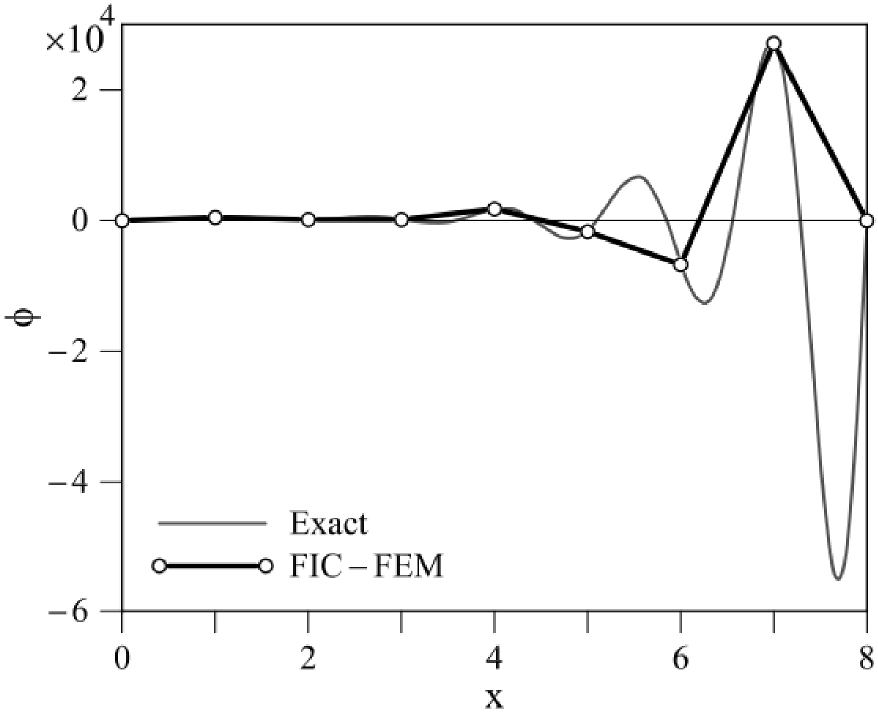
(b) $r_s - \frac{1}{2}h\frac{dr_s}{dx} = 0$

Space differential of the equation

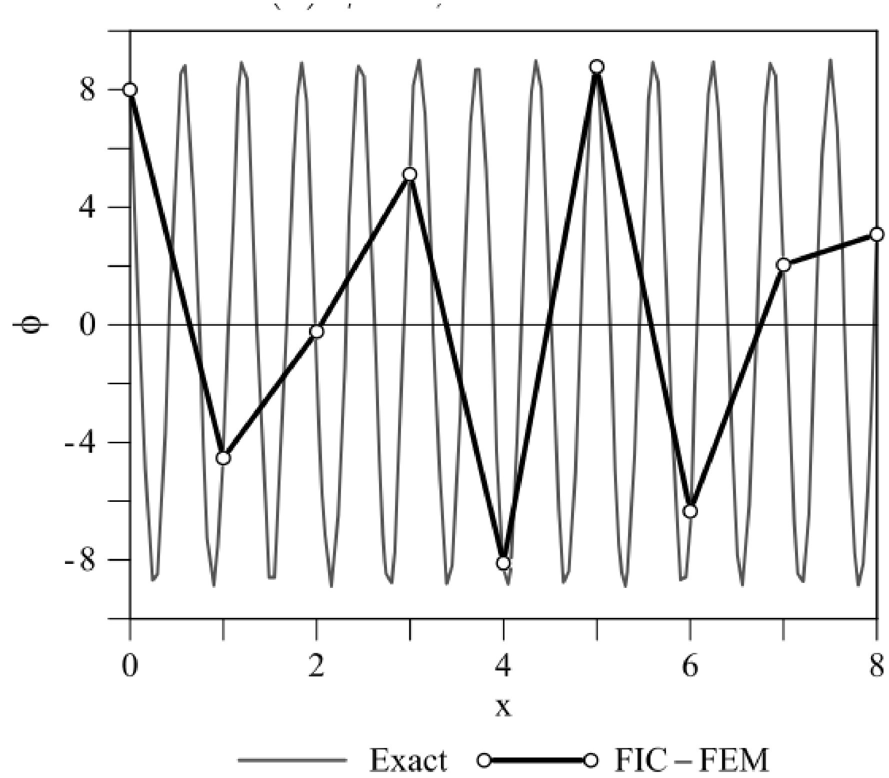
For advection equation,
point is the use of **phase information (=gradient) .**

Ex. of FIC results

(a) 1D convection-diffusion-production problem



(b)1D Helmholtz problem



FIC gives the very accurate solution on the very coarse grids.

Let's set a reference to the high accurate phase calculation method.

In this time, we use the conventional methods for advection : (Upwind) differencing scheme

Conventional Discretization method of advection term

Linear type(CFL-free form used by the Semi-Lagrangian scheme)

Upwind: 1st order

$$\phi_i^n = \phi_i^{n-1} + \frac{1}{2}\zeta_F\left(\phi_{id-s(c)} - \phi_{id}\right)$$

Lax-Wndroff: 2nd order

$$\phi_i^n = \phi_i^{n-1} + \frac{1}{2}\zeta_F\left\{(\zeta_F+1)\phi^{n-1}_{id-s(c)} - 2\phi^{n-1}_{id} + (\zeta_F-1)\phi^{n-1}_{id+s(c)}\right\}$$

QUICK: 2nd order

$$\phi_i^n = \phi_i^{n-1} + \frac{1}{8}\zeta_F\left\{-\phi^{n-1}_{id-2s(c)} + 7\phi^{n-1}_{id-s(c)} - 3\phi^{n-1}_{id} - 3\phi^{n-1}_{id+s(c)}\right\}$$

QUICKEST: 3rd order

$$\phi_i^n = \phi_i^{n-1} + \frac{1}{6}\zeta_F\left\{-(\zeta_F^2-1)\phi^{n-1}_{id-2s(c)} - 3(\zeta_F^2-\zeta_F-2)\phi^{n-1}_{id-s(c)} -3(-\zeta_F^2+2\zeta_F+1)\phi^{n-1}_{id} - (\zeta_F^2-3\zeta_F+2)\phi^{n-1}_{id+s(c)}\right\}$$

Upwind: 3rd order

$$\phi_i^n = \phi_i^{n-1} + \frac{1}{6}\zeta_F\left\{-\phi^{n-1}_{id-2s(c)} + 6\phi^{n-1}_{id-s(c)} - 3\phi_{id} - 2\phi^{n-1}_{id+s(c)}\right\}$$

Kawamura and Kuwahara: 3rd order

$$\phi_i^n = \phi_i^{n-1} + \frac{1}{6}\zeta_F\left\{-2\phi^{n-1}_{id-2s(c)} + 10\phi^{n-1}_{id-s(c)} - 9\phi^{n-1}_{id} + 2\phi_{id+s(c)} - \phi^{n-1}_{id+2s(c)}\right\}$$

Central : 4th order

$$\phi_i^n = \phi_i^{n-1} + \frac{1}{12}\zeta_F\left\{-\phi^{n-1}_{id-2s(c)} + 8\phi^{n-1}_{id-s(c)} - 8\phi^{n-1}_{id+s(c)} + \phi^{n-1}_{id+2s(c)}\right\}$$

Non linear type

TVD 3rd oeder

$$\partial_t\phi_i = -\Delta i\hat{f}$$

$$\hat{f}_{i+1/2} = \hat{f}^{(1)}_{i+1/2} + \frac{1}{4}c^+_{i+1/2}\left\{(1-k)\Psi(r^+_{i-1/2})\Delta\phi_{i-1/2} + (1+k)\Psi(r^-_{i+1/2})\Delta\phi_{i+1/2}\right\} - \frac{1}{4}c^-_{i+1/2}\left\{(1-k)\Psi(r^-_{i+3/2})\Delta\phi_{i+2/3} + (1+k)\Psi(r^+_{i+1/2})\Delta\phi_{i+1/2}\right\}$$

$$\hat{f}^{(1)}_{i+1/2} = \frac{1}{2}\left\{c^+_{i+1/2}\phi_i + c^-_{i+1/2}\phi_{i+1}\right\}$$

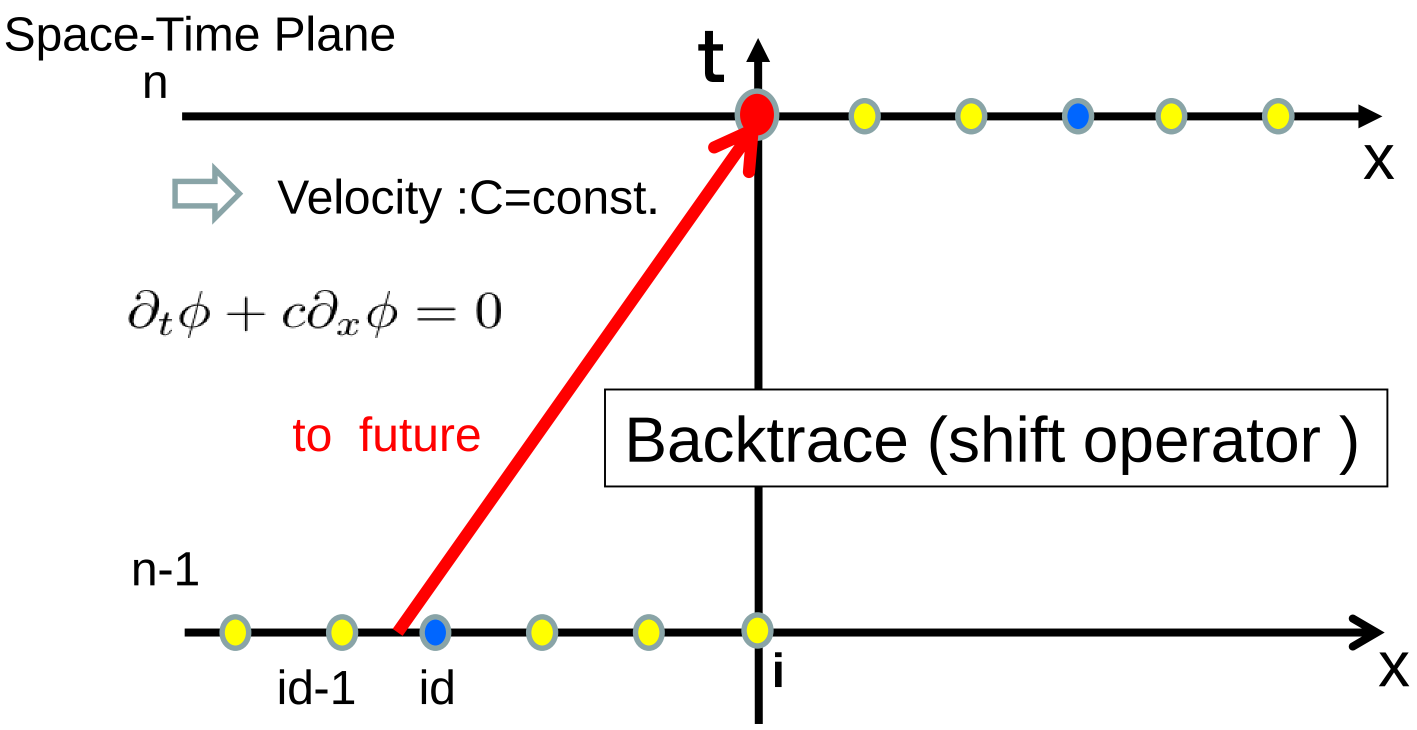
$$c^+_{i+1/2} = (c+|c|)_{i+1/2}, \quad c^-_{i+1/2} = (c-|c|)_{i+1/2}$$

PPM : Piecewise-Parabolic Method
ENO : Essentially Non-oscillatory
WENO: weighted **ENO**

$$\partial_t\phi + c\partial_x\phi = 0$$

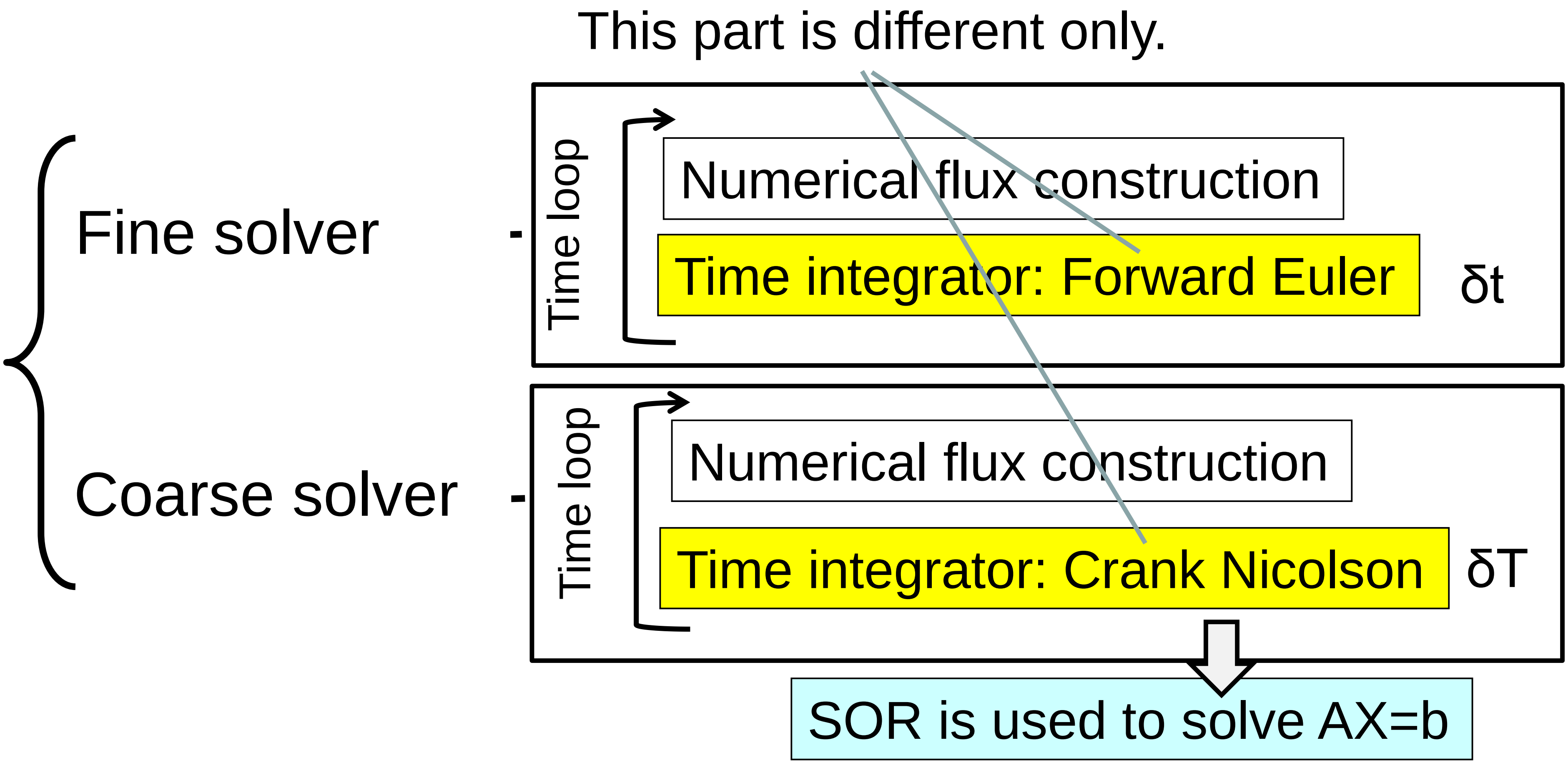
Semi-Lagrangian scheme

Considering the equation on the grid i



We choose the TVD scheme as conventional method and set Parareal_CN-TVD as reference.

Code of the coarse solver is same as one of the fine solver.



- δt: time step width of fine solver: set by the CFL condition: $\Delta x/v > \delta t$
- δT: time step width of coarse solver: $\delta T \gg \delta t$

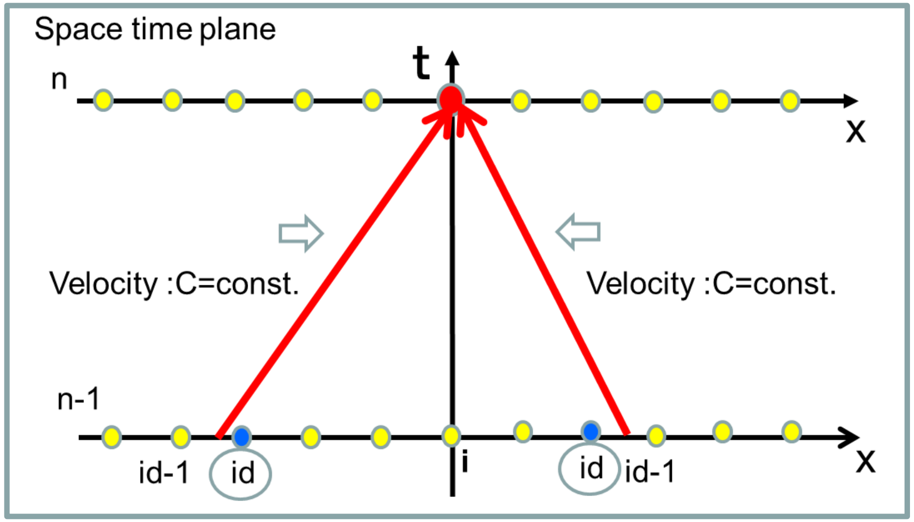
Impact of CIP Method on the parareal convegence.

CIP method

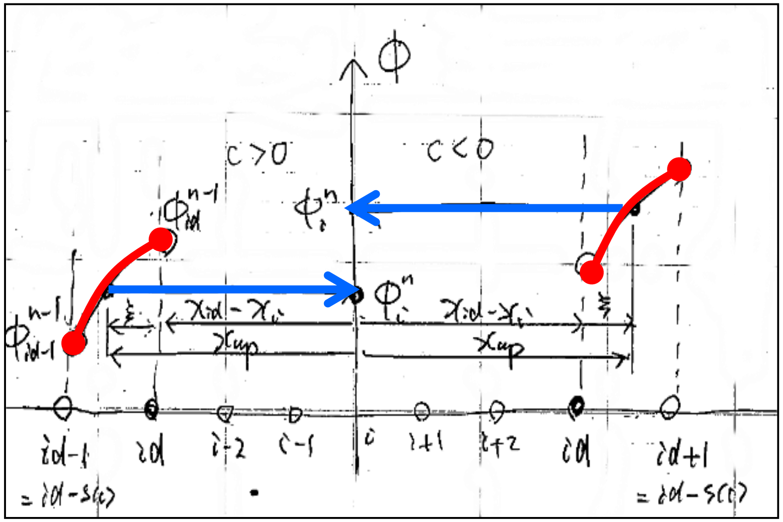
Up stream calculation and time integration is performed **by back-trace and shift operation** **(CFL free formula is used here.)**

＊Considering the equation on the grid i

Back-trace：



Shit operation



id = grid that is near i grid of cell (id, id-1)

$$id = i - \mathrm{INT}\left(\frac{\mathrm{x_u p}}{\Delta \mathrm{x}}\right) = \mathrm{i} - \mathrm{INT}\left(\frac{\mathrm{c}\delta \mathrm{t}}{\Delta \mathrm{x}}\right)$$

Back-trace points finding

$$\xi_F = x - x_{id} = x_i - c\delta t - x_{id} = -c\delta t - (x_i - x_{id}) = -c\delta t - \Delta x(i - id) = -c\delta t + \Delta x \mathrm{INT}\left(\frac{\mathrm{c}\delta \mathrm{t}}{\Delta \mathrm{x}}\right)$$

Upstream finding

$$D_F = -s(c)\Delta x, \quad s(c) = \mathrm{SIGN}(1.0, \mathrm{c})$$

Detail of Formula

CIP 3rd method

$$\partial_t \phi + c\partial_x \phi = 0$$
$$\partial_t g + c\partial_x g = 0$$
$$g = \partial_x \phi \quad \text{(gradient)}$$

CIP 5th method (We developed it as more accurate CIP at this time.)

$$\partial_t \phi + c\partial_x \phi = 0$$
$$\partial_t g + c\partial_x g = 0, \quad \partial_t \chi + c\partial_x \chi = 0 \quad \text{(gradient, curvature)}$$
$$g = \partial_x \phi, \quad \chi = \partial_x g$$

- **Space discretization： by the cubic interpolation function**

CIP 3rd method:

$$\phi(x) = F_{id}(x) = a_{id}(x - x_{id})^3 + b_{id}(x - x_{id})^2 + g_{id}(x - x_{id}) + \phi_{id}$$
$$g(x) = \partial_x F_{id}(x) = 3a_{id}(x - x_{id})^2 + 2b_{id}(x - x_{id}) + g_{id}(x - x_{id})$$

$$a_{id} = \frac{1}{D_F^3}\left\{-2(\phi_{id-s(c)} - \phi_{id}) + (g_{id-s(c)} + g_{id})D_F\right\}$$
$$b_{id} = \frac{1}{D_F^2}\left\{3(\phi_{id-s(c)} - \phi_{id})1(g_{id-s(c)} + 2g_{id})D_F\right\}$$

CIP 5th method:

$$\phi(x) = F_{id}(x) = a_{id}(x - x_{id})^5 + b_{id}(x - x_{id})^4 + c_{id}(x - x_{id})^3 + \chi_{id}/2(x - x_{id})^2 + g_{id}(x - x_{id}) + \phi_{id}$$
$$g(x) = \partial_x F_{id}(x) = 5a_{id}(x - x_{id})^4 + 4b_{id}(x - x_{id})^3 + 3c_{id}(x - x_{id})^2 + \chi_{id}(x - x_{id}) + g_{id}$$
$$\chi(x) = \partial_x^2 F_{id}(x) = 20a_{id}(x - x_{id})^3 + 12b_{id}(x - x_{id})^2 + 6c_{id}(x - x_{id}) + \chi_{id}$$

$$a_{id} = \frac{1}{D_F^5}\left\{6(\phi_{id-s(c)} - \phi_{id}) - 3(g_{id-s(c)} + g_{id})D_F + 1/2(\chi_{id-s(c)} - \chi_{id})D_F^2\right\}$$
$$b_{id} = \frac{1}{D_F^4}\left\{-15(\phi_{id-s(c)} - \phi_{id}) + 7(g_{id-s(c)} + 8/7 g_{id})D_F - (\chi_{id-s(c)} - 3/2\chi_{id})D_F^2\right\}$$
$$c_{id} = \frac{1}{D_F^3}\left\{10(\phi_{id-s(c)} - \phi_{id}) - 4(g_{id-s(c)} - 3/2 g_{id})D_F + 1/2(\chi_{id-s(c)} - 3\chi_{id})D_F^2\right\}$$

- **Up-date(time integration)： by Semi-Lagrange scheme**

CIP 3rd method:

$$\phi^n(x_i) = F_{id}^{n-1}(x_i - c\delta t)$$
$$g^n(x_i) = \partial_x F_{id}^{n-1}(x_i - c\delta t)$$

$$\phi^n(x_i) = a_{id}^{n-1}\xi_F^3 + b_{id}^{n-1}\xi_F^2 + g_{id}^{n-1}\xi_F^3 + \phi_{id}$$
$$g^n(x_i) = 3a_{id}^{n-1}\xi_F^2 + 2b_{id}^{n-1}\xi_F + g_{id}^{n-1}$$

CIP 5th method:

$$\phi^n(x_i) = F_{id}^{n-1}(x_i - c\delta t)$$
$$g^n(x_i) = \partial_x F_{id}^{n-1}(x_i - c\delta t)$$
$$\chi^n(x_i) = \partial_x^2 F_{id}^{n-1}(x_i - c\delta t)$$

$$\phi^n(x_i) = a_{id}^{n-1}\xi_F^5 + b_{id}^{n-1}\xi_F^4 + c_{id}^{n-1}\xi_F^3 + \chi_{id}/2\xi_F^2 + g_{id}\xi_F + \phi_{id}$$
$$g^n(x_i) = 5a_{id}^{n-1}\xi_F^4 + 4b_{id}^{n-1}\xi_F^3 + 3c_{id}^{n-1}\xi_F^2 + \chi_{id}\xi_F + g_{id}^{n-1}$$
$$\chi^n(x_i) = 20a_{id}^{n-1}\xi_F^3 + 12b_{id}^{n-1}\xi_F^2 + 6c_{id}^{n-1}\xi_F + \chi_{id}$$

Code of CIP-5th method

Set of the advection parameters

Calculation of the coefficient of spline function

Update of variables

```
do j=1,Ny; do i=1,Nx
     cx   =0.5d0*(v1(i-1,j,1)+v1(i,j,1))
     ida =i-int(cx*dt/dx)
     xgi =-cx*dt+dx*real(i-ida)
     ais =sign(1.0,cx)
     idam=ida-int(ais)
     fv   =               v1(ida,j,3)
     gfi =gf (ida,j,1) !  dfai/dx
     ggfi=ggf(ida,j,1) ! ddfai/dx/dx
     dfi =v1 (idam,j,3)-v1(ida,j,3)
     aid1=-dx5*ais*(  6.0* dfi &
    &               + 3.0*(    gf (idam,j,1)+     gfi)*dx*ais  &
    &               + 0.5*(    ggf(idam,j,1)-    ggfi)*ddx     )
     bid1= dx4*    (-15.0* dfi &
    &               -      (7.0*gf (idam,j,1)+8.0* gfi)*dx*ais  &
    &               -      (    ggf(idam,j,1)-1.5*ggfi)*ddx     )
     cid1=-dx3*ais*( 10.0* dfi &
    &               + 4.0*(    gf (idam,j,1)+1.5* gfi)*dx*ais  &
    &               + 0.5*(    ggf(idam,j,1)-3.0*ggfi)*ddx     )
     v2  (i,j,3)= &
   &((((     aid1*xgi+     bid1)*xgi+    cid1)*xgi+0.5*ggfi)*xgi+gfi)*xgi+fv
     gfn (i,j,1)= &
   & ((( 5.0*aid1*xgi+ 4.0*bid1)*xgi+3.0*cid1)*xgi+    ggfi)*xgi+gfi
     ggfn(i,j,1)= &
   &  ((20.0*aid1*xgi+12.0*bid1)*xgi+6.0*cid1)*xgi+    ggfi
end do; end do
```

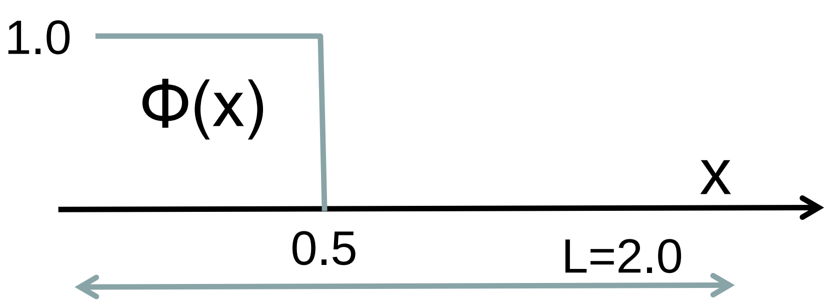
CIP-5th method is very simple and we can easily develop CIP-5th code based on CIP-3rd method code.

Check performance of the CIP-5th method by comparing the CIP-3rd and CIP-5th methods

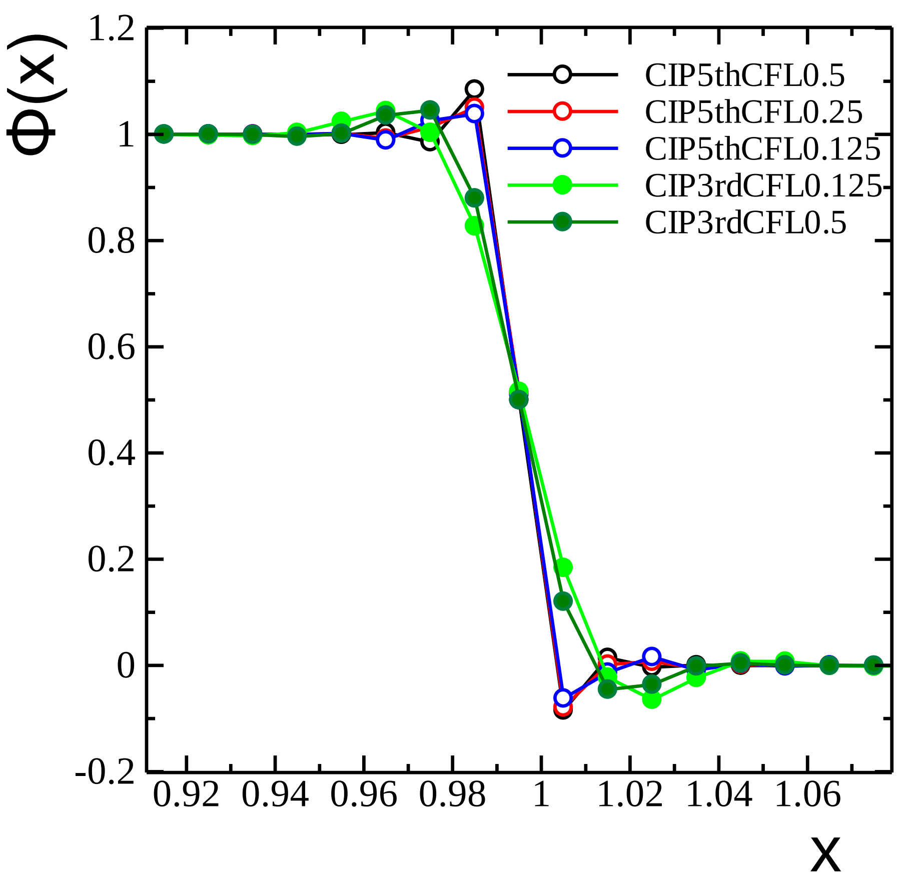
Case-1: Advection of step shape

(a) test parameters

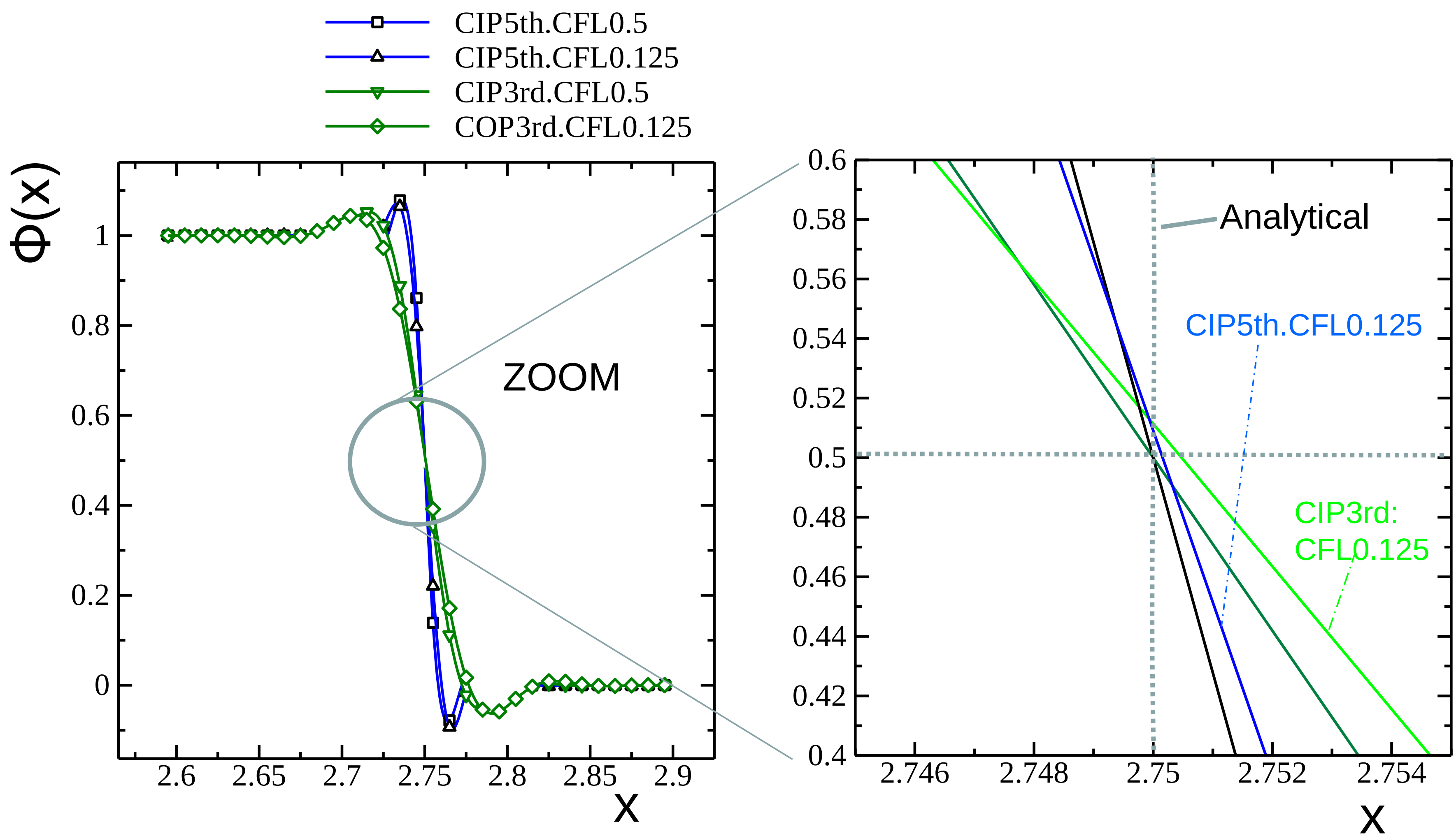
- Physical condition
  - 1D convection of step shape
    - Speed: c=1
  - Space length : L=2
  - Time length : **T=0.5、2.0**
- Numerical analysis condition
  - Num. of meshes: 200
    → dx=0.01
  - Width of time step
    → dt=0.005,0.0025,0.00125
    → CFL=0.5, 0.25, 0.125
  - Initial condition
    → x=0--0.5:Φ=1.0, x > 0.5: Φ=0.0



(b) Results of Φ distribution (t=0.5)



(c) Results of Φ distribution (t=2.0)　　(c’) Zoomed part



CIP-5th method → Width of step is thinner.

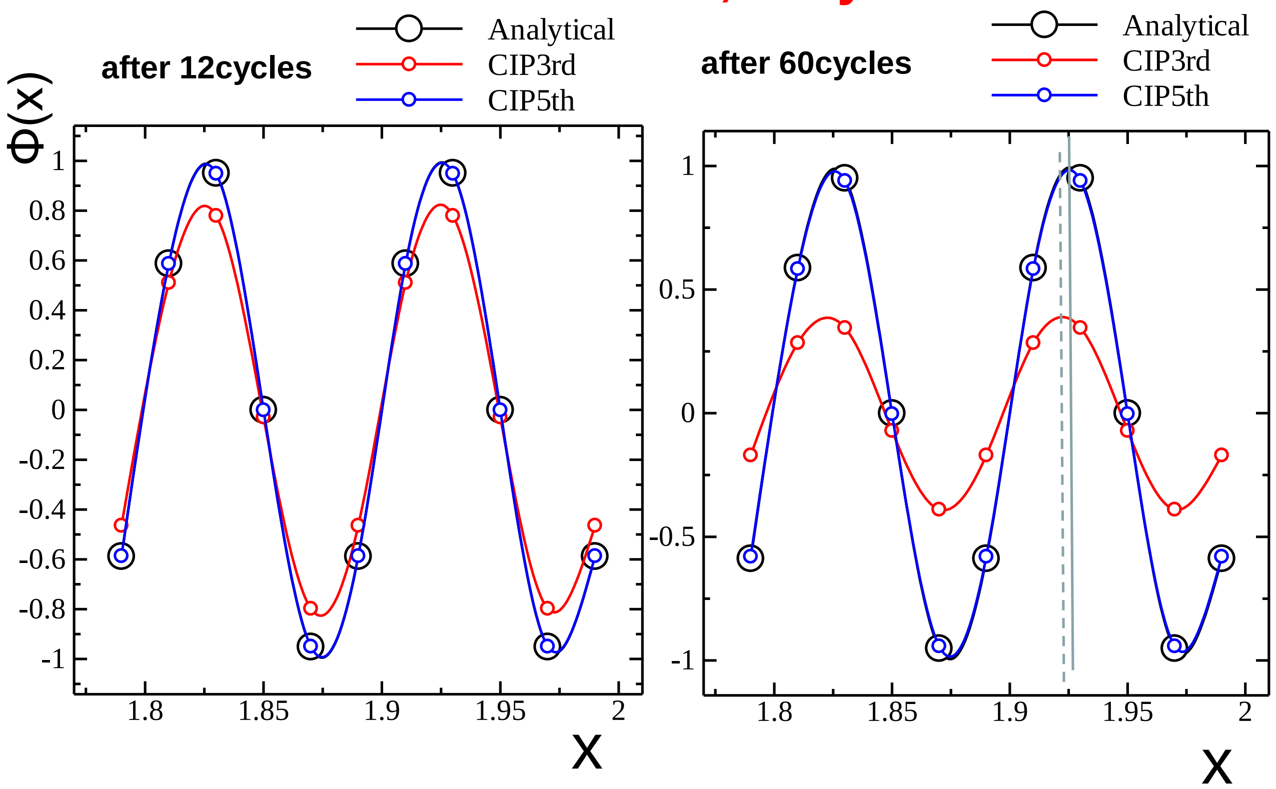
→ Phase accuracy is better.

Case-2: Advection of sin wave

(a) test parameters

- Physical condition
  - 1D convection of sin wave
    - Speed c=1
  - Space length : L=2
  - Time length : **T=0.6、3.0**
- Numerical analysis condition
  - Num. of meshse: 100
    → dx=0.02
  - Width of time step
    → dt=0.015→CFL=0.75
    → **one wave/5grids**
  - Initial condition
    → **Sin wave**

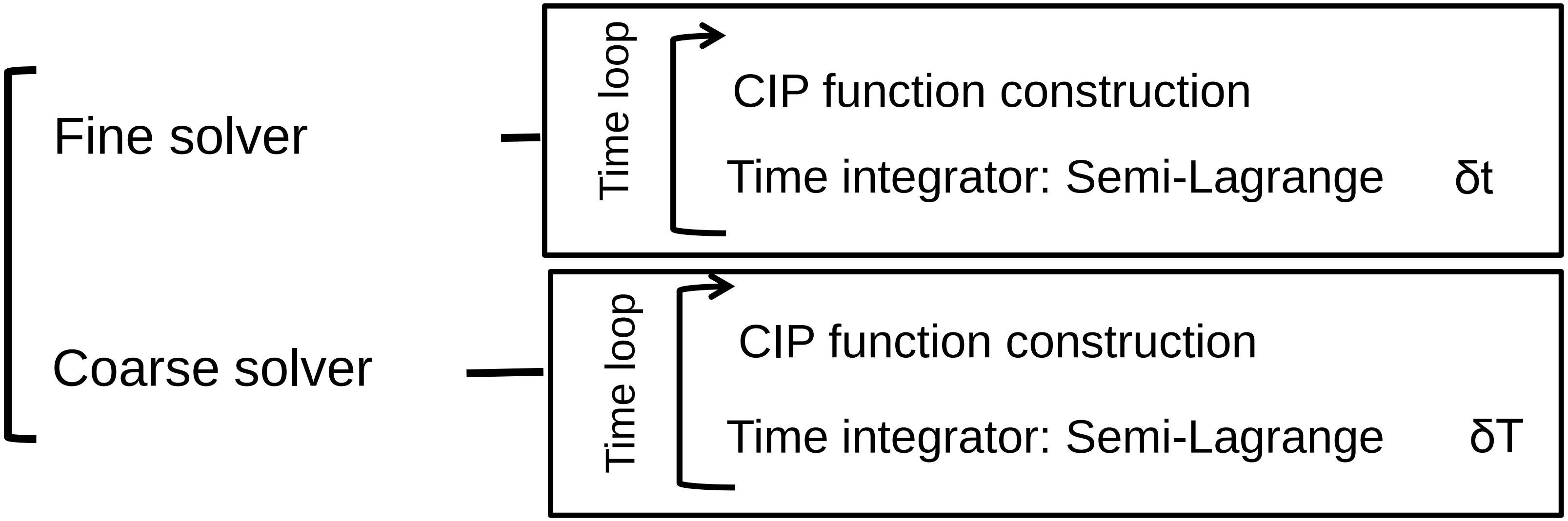
(b) Φ distribution (after 12, 60cycles)



CIP-5th → Damping of amplitude is very smaller .
→ Phase accuracy is better.

Let's study the impact of CIP-5th on the parareal iteration!

Parareal_CIP (3rd, 5th)



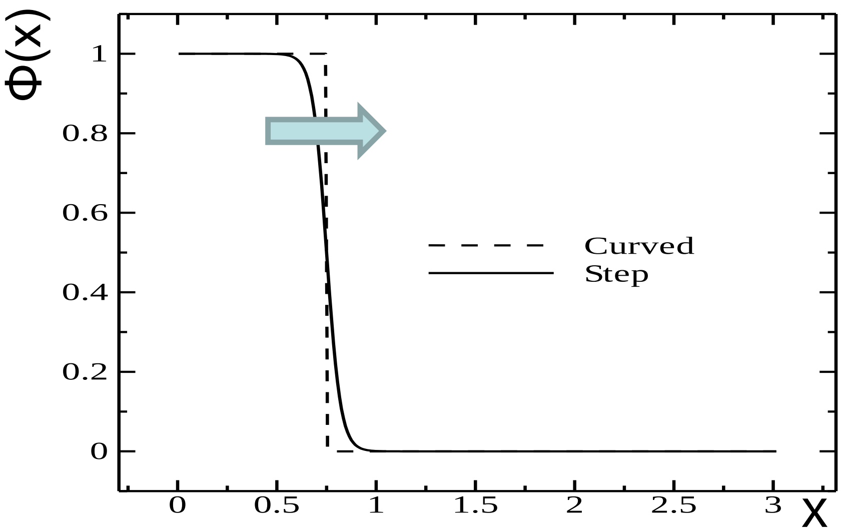
- δt: time step width of fine solver: fixed by the CFL condition: $\Delta x/v < \delta t$
- δT: time step width of coarse solver: $\delta T \gg \delta t$

Flow of Parareal_CIP is same for CIP-3rd and CIP-5th methods.

Numerical test: Parameters

Test problem	● **C = 1.0 and Space [0,3] × Time: [0, 2.0]** ● **(a) advection of step shape** ● **(b) advection of step like wave** f(x)=0.5(1-tanh((x-xo)/xi)、 xi : width of step → xo=1.0, → xi =SQRT(2D/k)=SQRT(2/k): 0.035(k=1600),0.07(k=400) } See the initial condition bellow.
Space and time descritaization	● dx=0.01, 200meshes (10grids/wave) →L=dx × 200=2 ● δt =0.001(CFL=0.1) ● Boundary condition ： continuous
PinT condition	● Number of time slices: 20 ● Rfc = 25 (δT= 0.025)

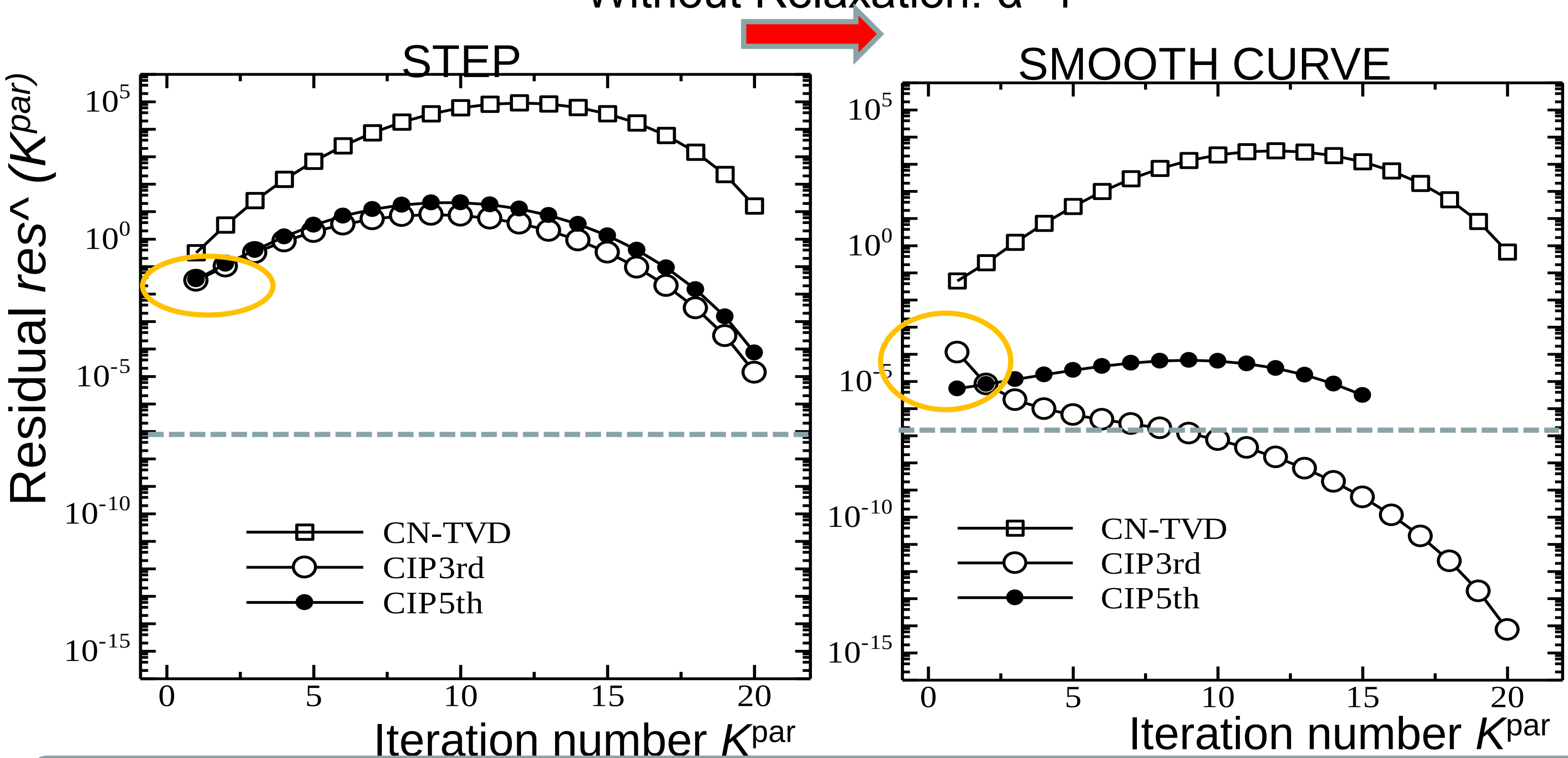
Initial condition



"Step" and "Smooth curves" are used as initial condition.
→ When smoothness of curve increases, the number of high wave number waves decrease in curves.

Residual during the parareal iteration: Influence of CIP5th and reducing the number of high wave number waves

Without Relaxation: α=1



Relaxation parameter α < 1.0

$$\mathbf{U}_n^k = F(T_n, T_{n-1}, \mathbf{U}_{n-1}^{k-1}) + \alpha \left\{ G(T_n, T_{n-1}, \mathbf{U}_{n-1}^{k}) - G(T_n, T_{n-1}, \mathbf{U}_{n-1}^{k-1}) \right\}$$

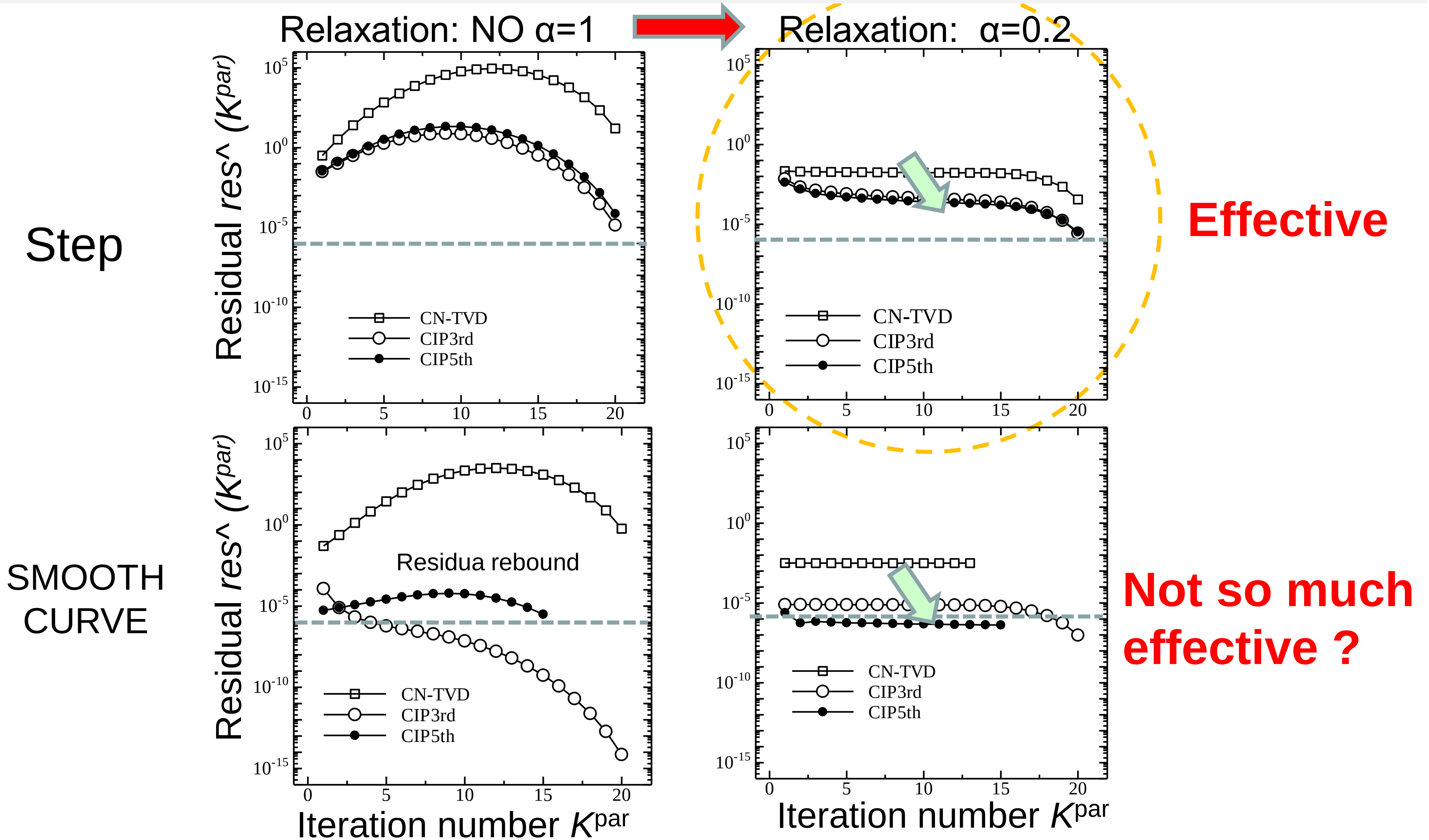
∗ CIP method and reduce of the number of high wave number waves improves the convergence.

∗ CIP 5th has not so much effectiveness than CIP3rd.

→ Reason why not yet clear ?

Residual during the parareal iteration

Influence of parareal iteration realxation

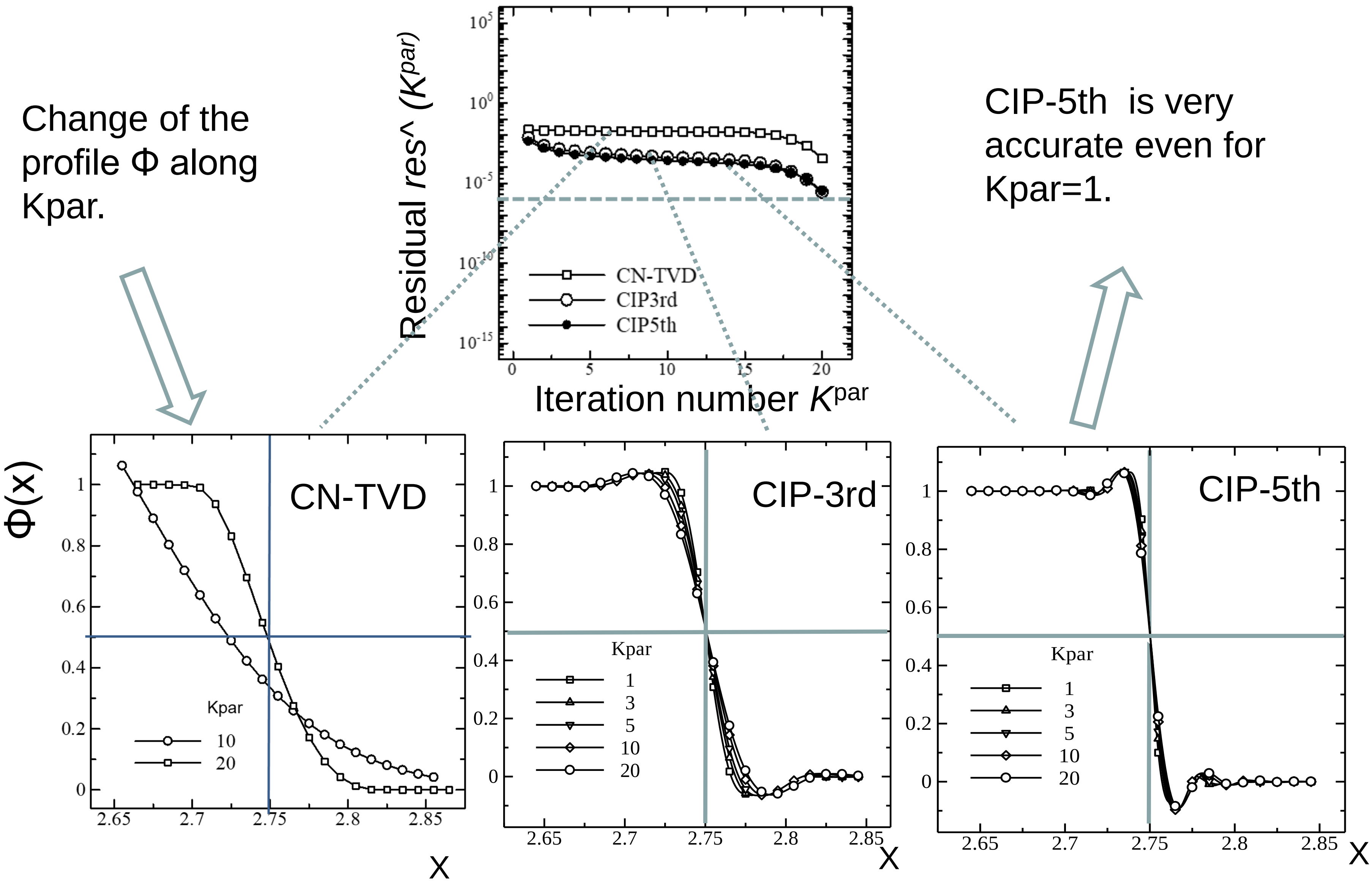


Relaxation is effective for residual rebound, but case by case.

CIP-5th looks not so much effective than CIP-3rd, really ? Then, check the profile of variable along iteration･･･

Change of the profile Φ along Kpar.

CIP-5th is very accurate even for Kpar=1.

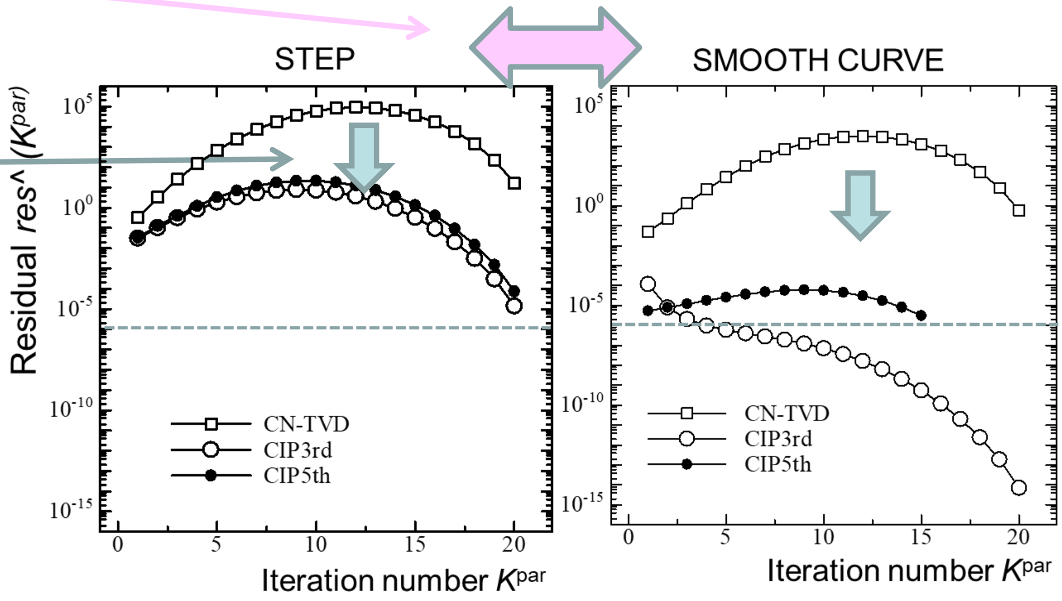


Profile show that CIP-5th is effective even for first sate of the iteration!

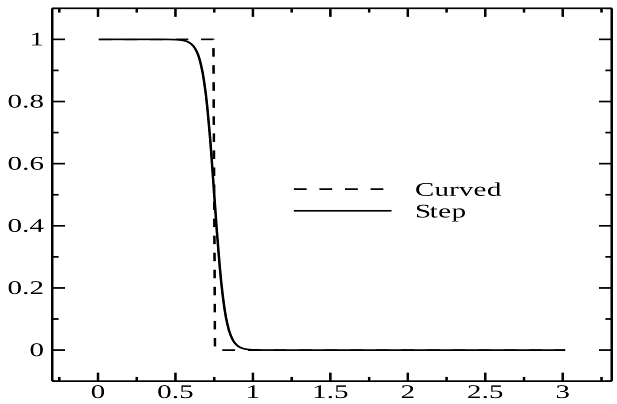
Summary and Future Work

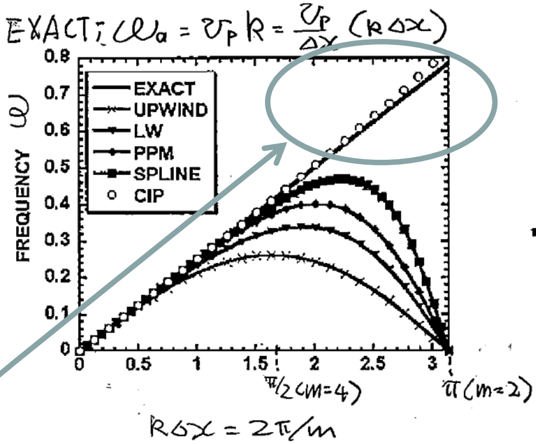
Summary:

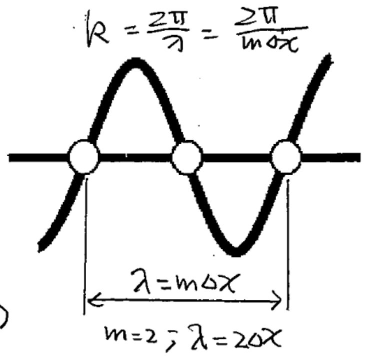
- **Increasing the accuracy of phase calculation by the CIP method is effective for improvement of parereal convergence.**
  - **High wave number modes cause the difficulty of pararel convergence via decreasing accuracy of phase calculation.**



- **Parareal algorithm should be evaluated using step convection problem to dig up issues.**







- **Phase of high wave number modes tends to become worse by the numerical damping even if we use the CIP method.**

Then, the improvement of the CIP3rd, 5th is need.

Future work

Conventional main method

Methods that are tried in this study

(1) CIP scheme: advecting the phase information by the gradient of value Φ.

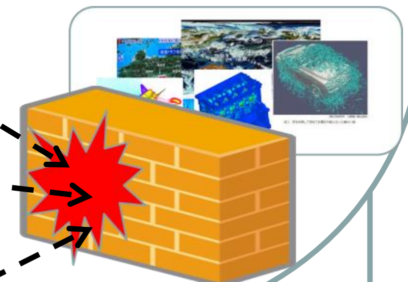
(A) Next, We try to combination of STRS scheme and CIP method.
(B) Control of the residual rebound

$$\partial_t \phi + c\partial_x \phi = 0$$

$$\partial_t g + c\partial_x g = 0$$
$$g = \partial_x \phi$$

Main issue : Gap of phase accuracy between fine and coarse solver

not enough



(3)Hybrid STRS-CIP

not yet success

Stabilization:
numerical damping
Accuracy:
Space and time higher order terms

$$\partial_{t'} \phi + c\partial_{x'} \phi = 0$$

There is a limit in the use.

(2) STRS scheme: achieving the stabilization and error elimination using "space and time reversal symmetry".

See you next in Roscoff Marine Station, Frace at May, PinT 2018 meeting.