Numerics and Boundary Conditions (used in PALM)

PALM group

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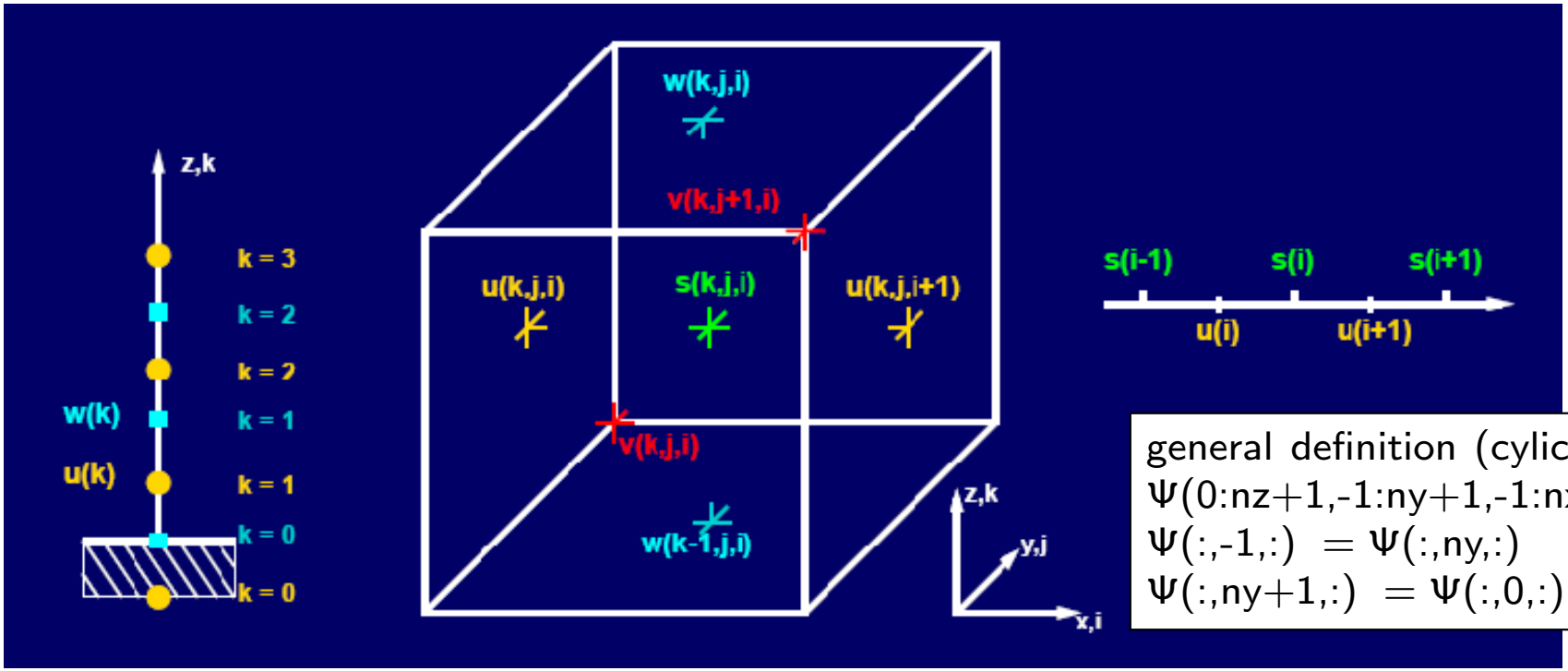
- **Lagrangian particle model included**
- **Boundary conditions:**
  - Cyclic and non-cyclic horizontal boundary conditions
  - Surface layer with Monin-Obukhov similarity
  - Topography
  - Turbulent inflow (for non-cyclic horizontal boundary conditions)

Numerical Grid



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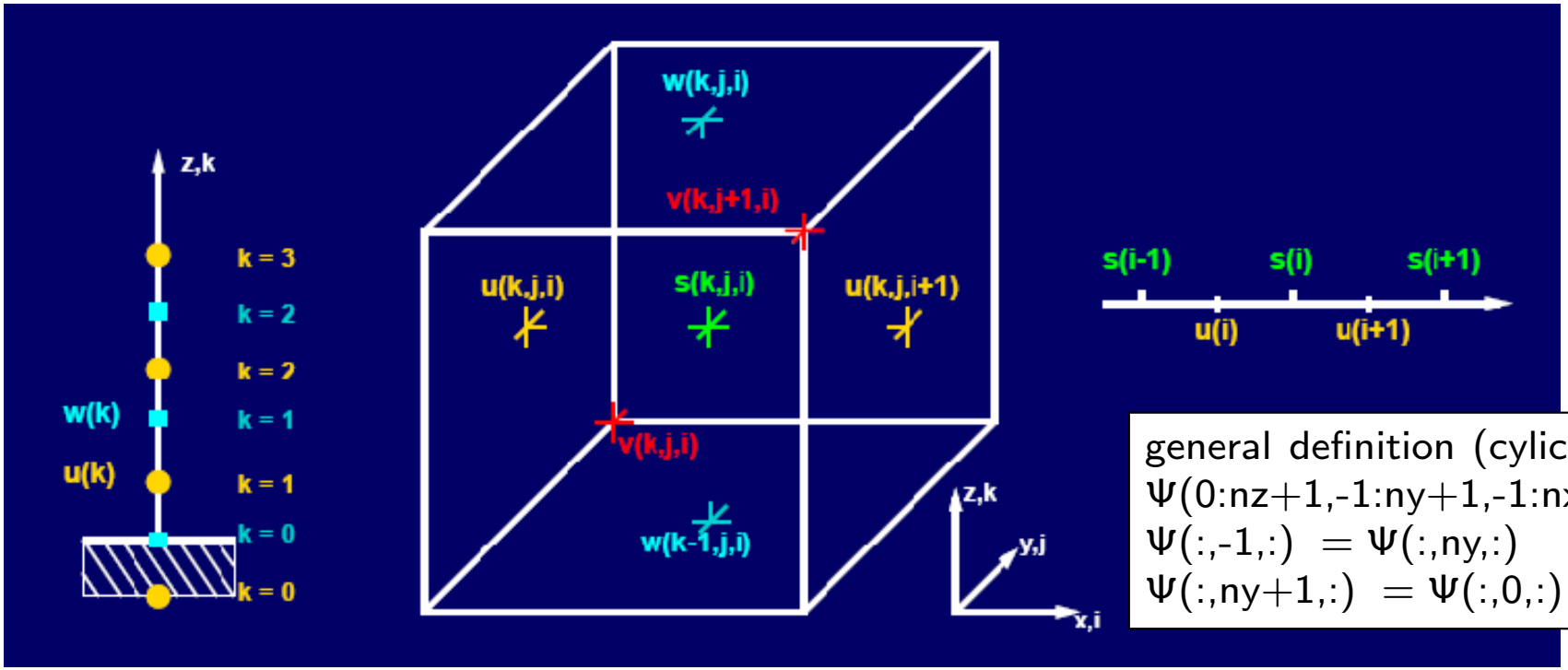

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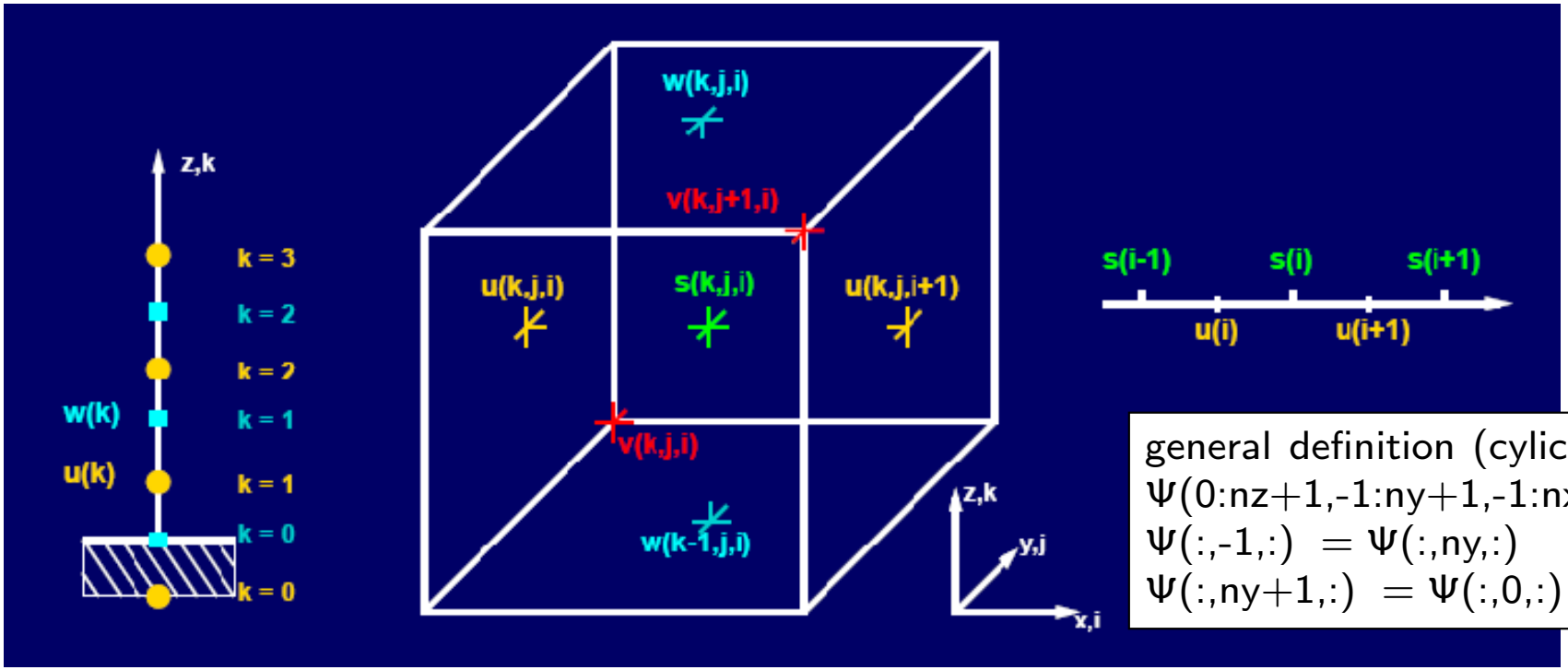

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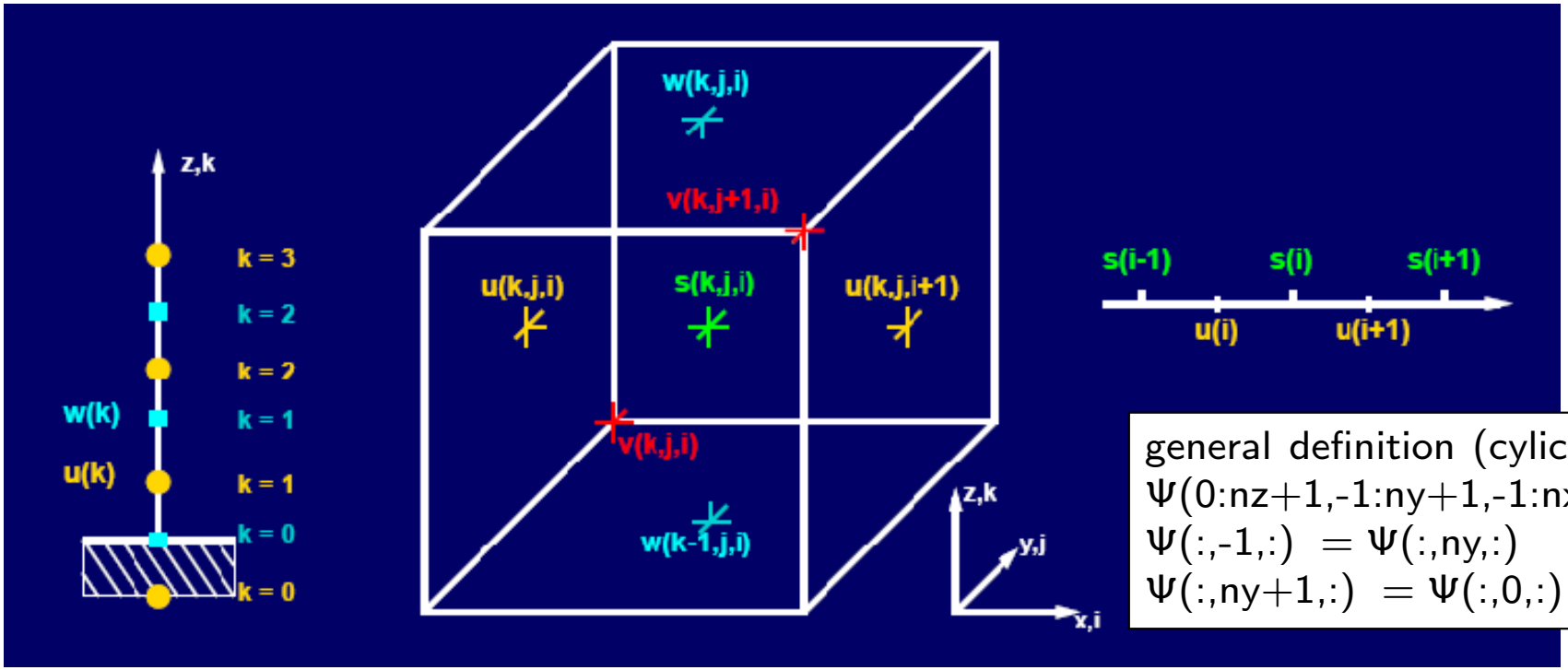

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- All scalar variables s (e.g. , p^*, e, K_m, K_h) are defined at the cell centers.
- Velocity components (u, v, w) are shifted by half of the grid spacing.
- Spacings are equidistant, stretching along z is possible.

Timestep Methods (I)

- **Euler**

$$\frac{\partial \psi(t)}{\partial t} = F(\psi(t)) \rightarrow \frac{\psi(t+\Delta t) - \psi(t)}{\Delta t} \approx F(\psi(t))$$

$$\psi(t+\Delta t) = \psi(t) + \Delta t \cdot F(\psi(t)) \qquad \mathcal{O}(\Delta t)$$

(used for SGS-TKE in special cases)

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- **Runge-Kutta, third-order**

$$k_1 = F(\psi(t))$$
$$k_2 = F\left(\psi(t) + \tfrac{1}{3}\Delta t \cdot k_1\right)$$
$$k_3 = F\left(\psi(t) - \tfrac{3}{16}\Delta t \cdot k_1 + \tfrac{15}{16}\Delta t \cdot k_2\right)$$
$$\psi(t+\Delta t) = \psi(t) + \tfrac{1}{30}\Delta t(5k_1 + 9k_2 + 16k_3) \qquad \mathcal{O}(\Delta t^2) \qquad C \leq 0.9$$

Timestep Methods (II)

In the PALM code, the different timestep schemes are treated by one equation using switches:

$$\psi(t+\Delta t) = (1-c_1)\cdot\psi(t-\Delta t)+c_1\cdot\psi(t)+\Delta t\cdot[c_2\cdot F(\psi(t)) + c_3\cdot F(\psi(t-\Delta t))]$$

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Scheme	$\mathbf{c}_1$	$\mathbf{c}_2$	$\mathbf{c}_3$
Euler	1	1	0
RK (1st step)	1	1/3	0
RK (2nd step)	1	15/16	-25/48
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$$\psi(t-\Delta t) = \psi(t) \qquad \textbf{after each RK substep}$$
$$\psi(t) = \psi(t+\Delta t)$$

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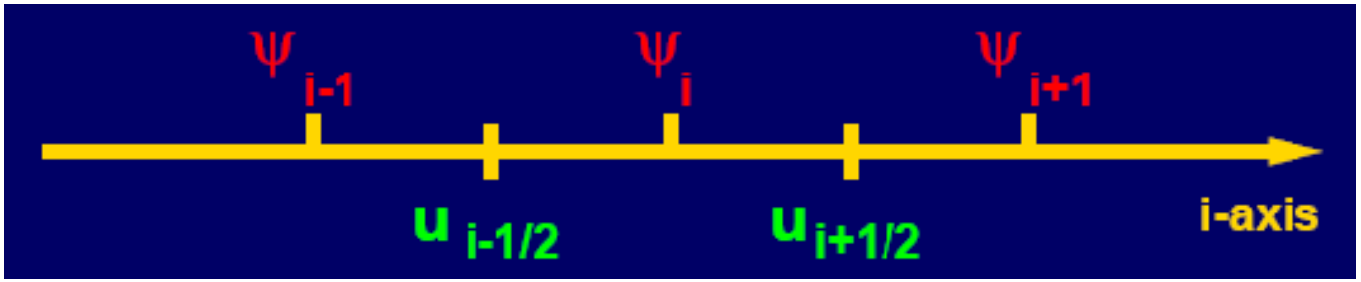

$$\left.\frac{\partial(u\psi)}{\partial x}\right|_i = \frac{1}{2\Delta x}\left(u_{i+\frac{1}{2}}\psi_{i+1} - u_{i-\frac{1}{2}}\psi_{i-1}\right)$$

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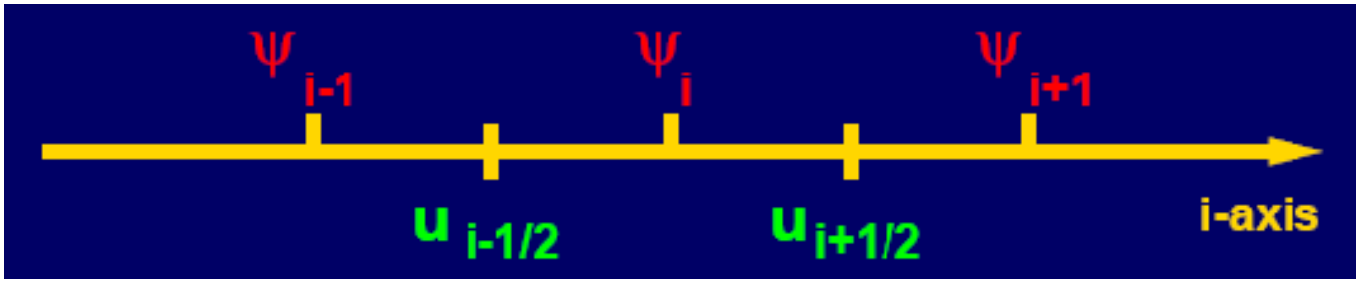

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- In case of momentum advection (e.g. $\psi = u$), u_{i-1} and u_{i+1} have to be obtained by linear interpolation.
- May cause $2\Delta x$ wiggles in case of sharp gradients.

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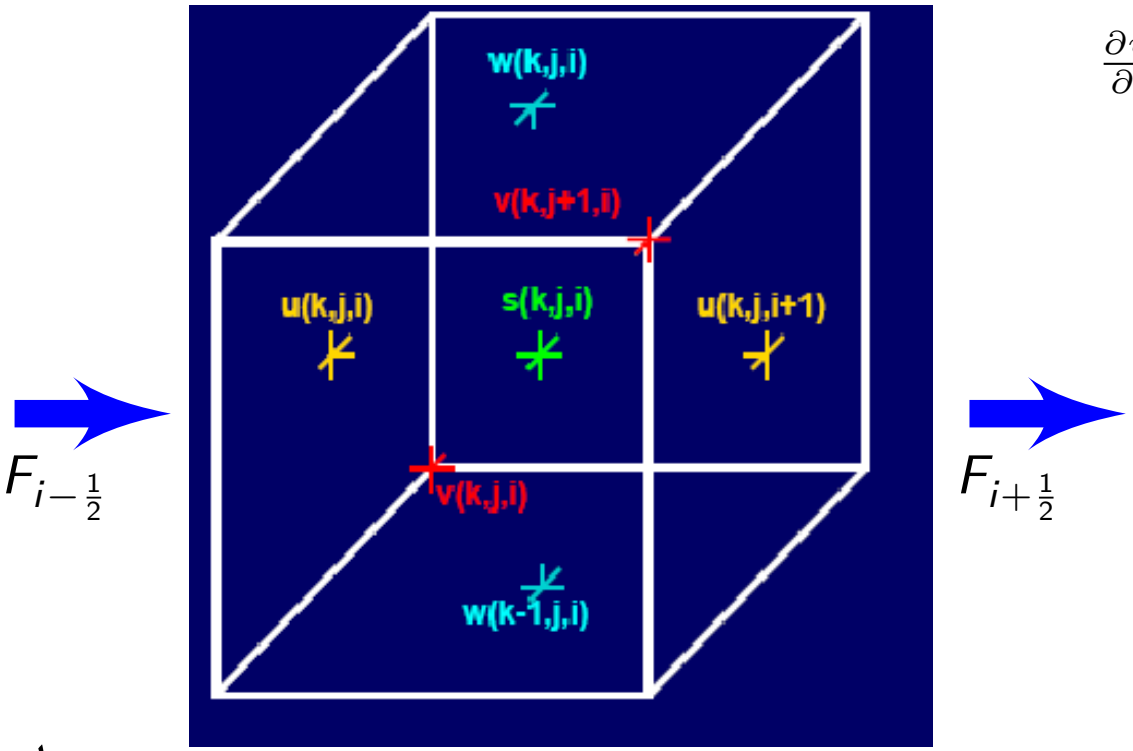
  - Adds additional numerical dissipation

Advection Methods – Wicker/Skamarock (I)

- Wicker and Skamarock (2002, Mon. Wea. Rev. 130, 2088 – 2097).
- Based on flux form of advection term
- Difference of fluxes at the edge of the grid cell is used to discretise advection term



$$\frac{\partial \psi}{\partial t} = -\nabla(u_i \psi) \approx -\frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta x}$$

Advection Methods – Wicker/Skamarock (II)

Finite difference approximation of 6^{th} order

$$F^{6\text{th}}_{i-\frac{1}{2}} = \frac{1}{60} u_{i-\frac{1}{2}} \left(37(\Psi_i + \Psi_{i-1}) - 8(\Psi_{i+1} + \Psi_{i-2}) + (\Psi_{i+2} + \Psi_{i-3})\right)$$

Artificially added numerical dissipation term

$$-\frac{1}{60} \left| u_{i-\frac{1}{2}} \right| \left(10(\Psi_i - \Psi_{i-1}) - 5(\Psi_{i+1} - \Psi_{i-2}) + (\Psi_{i+2} - \Psi_{i-3})\right)$$

Advection Methods – Wicker/Skamarock (III)

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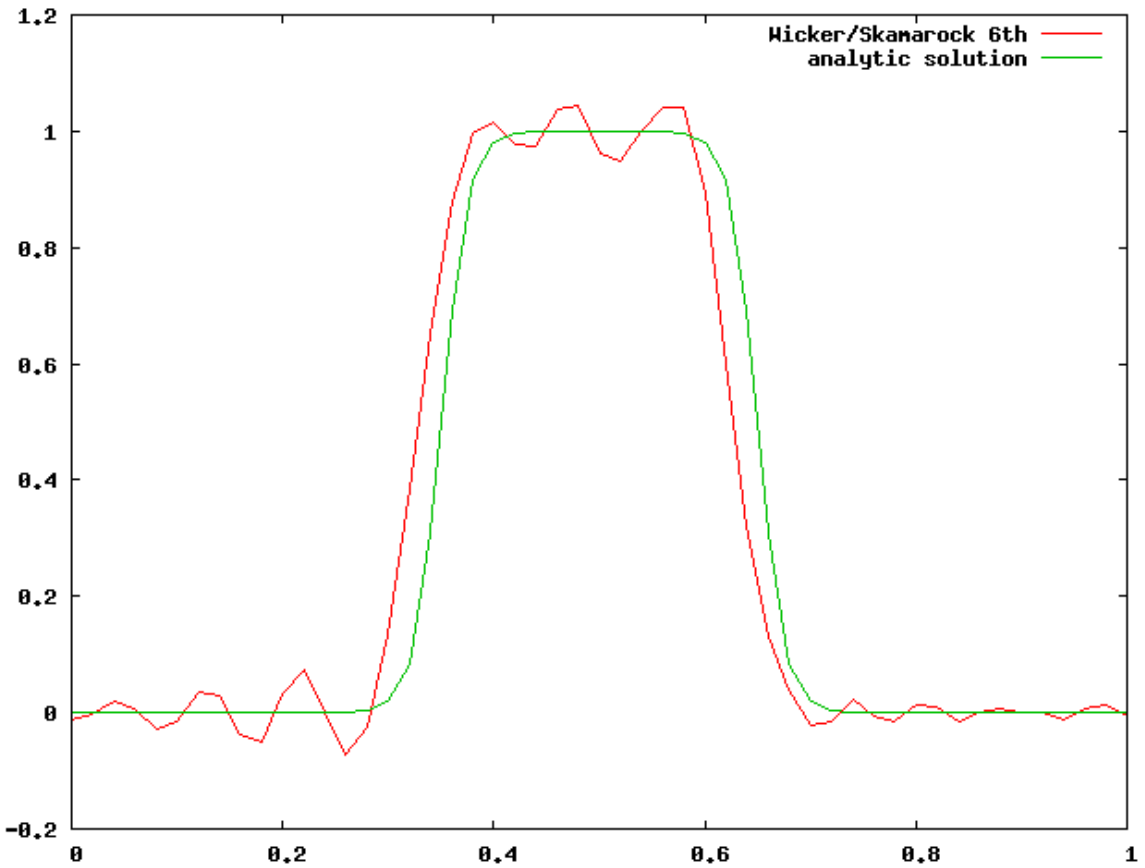
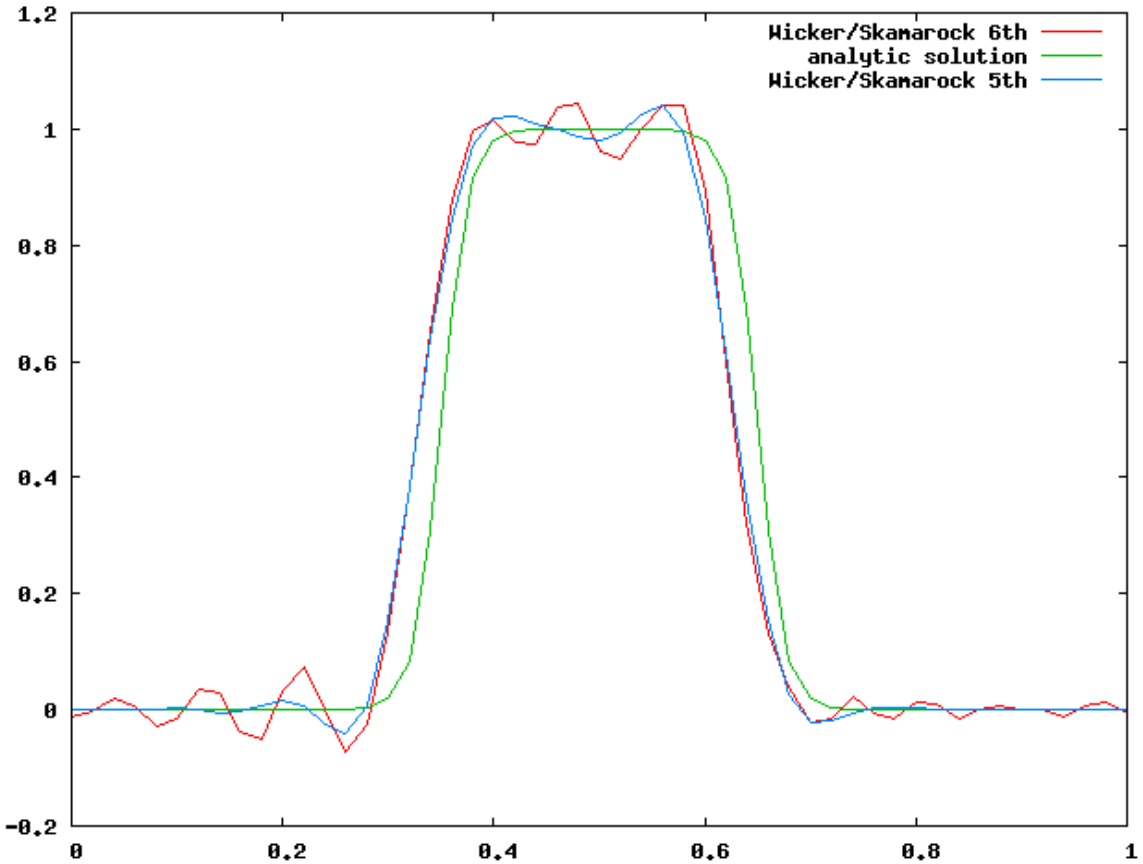


Centered Finite Differences produces numerical oscillations ("wiggles") near sharp gradients.

Advection Methods – Wicker/Skamarock (IV)

$$F^{5th}_{i-\frac{1}{2}} = F^{6th}_{i-\frac{1}{2}} - \frac{1}{60}\left|u_{i-\frac{1}{2}}\right|\left(10(\Psi_i - \Psi_{i-1}) - 5(\Psi_{i+1} - \Psi_{i-2}) + (\Psi_{i+2} - \Psi_{i-3})\right)$$



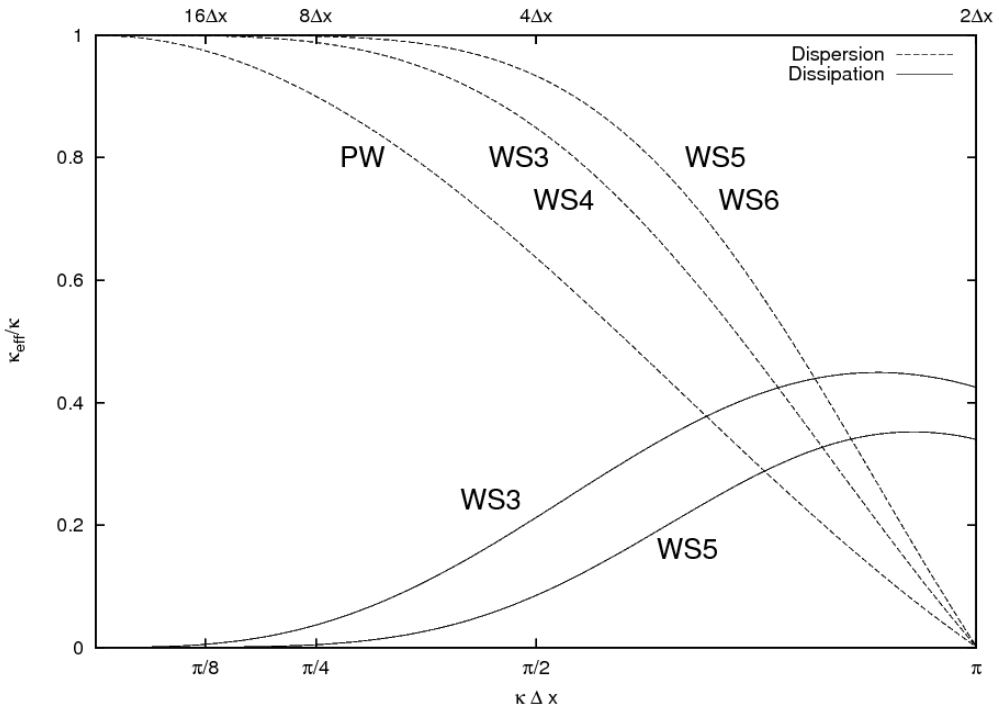
Advantage

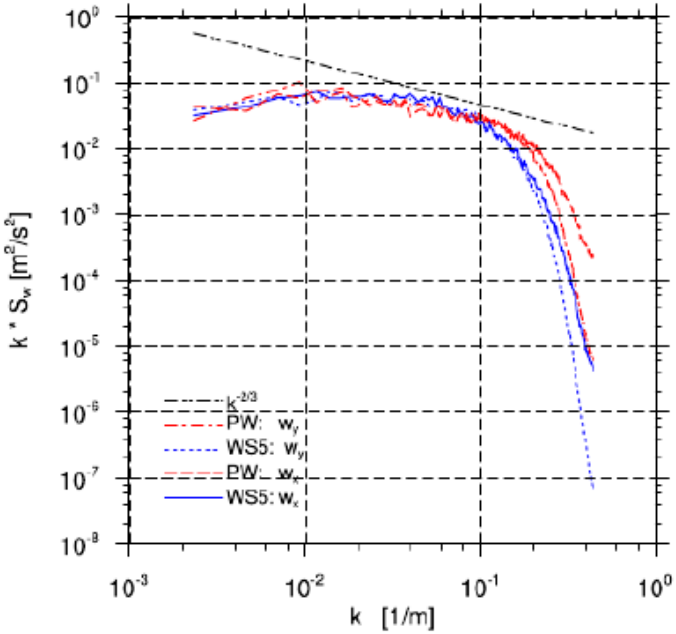
Numerical Dissipation damps small scale oscillations.

Disadvantage

In a turbulent flow numerical dissipation removes energy from small scales.

Advection Methods – Wicker/Skamarock (V)





- Better resolution of larger scales ($> 8\,\Delta x$) and hence less numerical energy transfer from larger to smaller scales compared to lower order schemes.
- Less spectral energy at smaller scales.

Pressure Solver (I)

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- Incompressibility is reached by a predictor-corrector method
  1. Momentum equations are solved without the pressure term giving a provisional velocity field which is not free of divergence.

$$\overline{u}_{i_{\mathrm{prov}}}^{t+\Delta t} = \overline{u}_i^t + \Delta t \left(-\frac{\partial}{\partial x_k} \overline{u}_k^t \overline{u}_i^t - (\varepsilon_{ijk} f_j \overline{u}_k^t - \varepsilon_{i3k} f_3 u_{g_k}) + g \frac{\overline{\theta^*}^t}{\theta_0} \delta_{i3} - \frac{\partial}{\partial x_k} \overline{u_k' u_i'}^t \right)$$

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2. Assign all remaining divergences to the (perturbation) pressure p^* so that the new corrected velocity field is the sum of the provisional, divergent field and the perturbation pressure term.

$$\overline{u}_i^{t+\Delta t} = \overline{u}_{i_{\mathrm{prov}}}^{t+\Delta t} + \Delta t \left(-\frac{1}{\rho_0} \frac{\partial \overline{p^*}^t}{\partial x_i} \right)$$

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3. The divergence operator is applied to this equation. Demanding a corrected velocity field free of divergence, this leads to a Poisson equation for the perturbation pressure.

$$\frac{\partial^2 \overline{p^*}^t}{\partial x_i^2} = \frac{\rho_0}{\Delta t} \frac{\partial \overline{u}_{i_{\mathrm{prov}}}^{t+\Delta t}}{\partial x_i}$$

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4. After solving the Poisson equation, the final velocity field is calculated as given in step 2.

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- FFT-solver
  1. Discretization of the Poisson-equation by central differences

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  - Requires periodic boundary conditions and uniform grids along x and y

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- Multigrid-method
  - Iterative solver
    basic idea: Poisson equation is transformed to a fixed point problem:
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$$\begin{aligned} \vec{p}^{1} &= T \cdot \vec{p}^{0} + \vec{c}^{0} \\ \vec{p}^{2} &= T \cdot \vec{p}^{1} + \vec{c}^{1} \\ &\vdots \\ \vec{p}^{k} &= T \cdot \vec{p}^{k-1} + \vec{c}^{k-1} \\ \vec{p}^{k+1} &= T \cdot \vec{p}^{k} + \vec{c}^{k} \end{aligned}$$

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  - With each iteration step k the improved solution converges towards the exact solution.
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  - Very low convergence: $\mathcal{O}(n^2)$.

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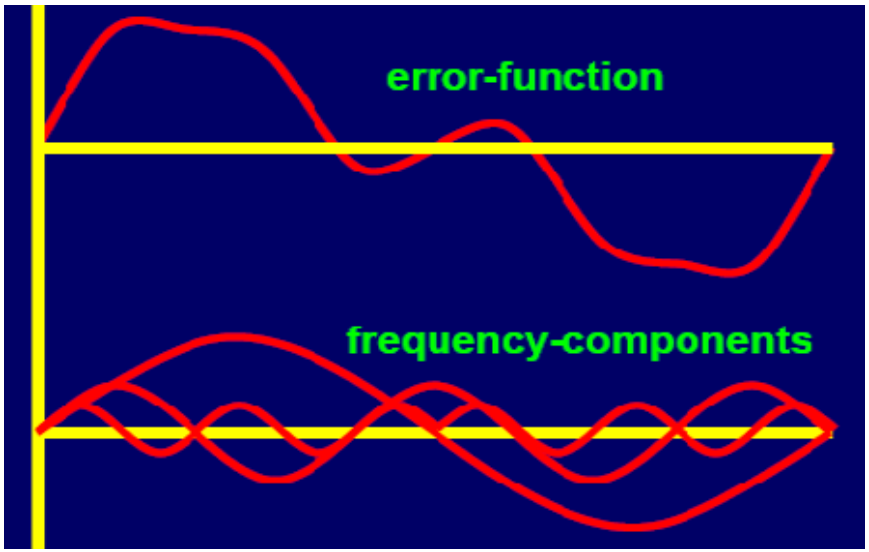
  - Due to their locality, iterative solvers show a frequency-dependent reduction of the residual: low frequencies are reduced slower than high frequencies.
  - The main idea of the multigrid method is to reduce errors of different frequencies on grids with different grid spacing:
    - errors of high frequency are reduced on fine grids
    - errors of low frequency are reduced on coarse grids.



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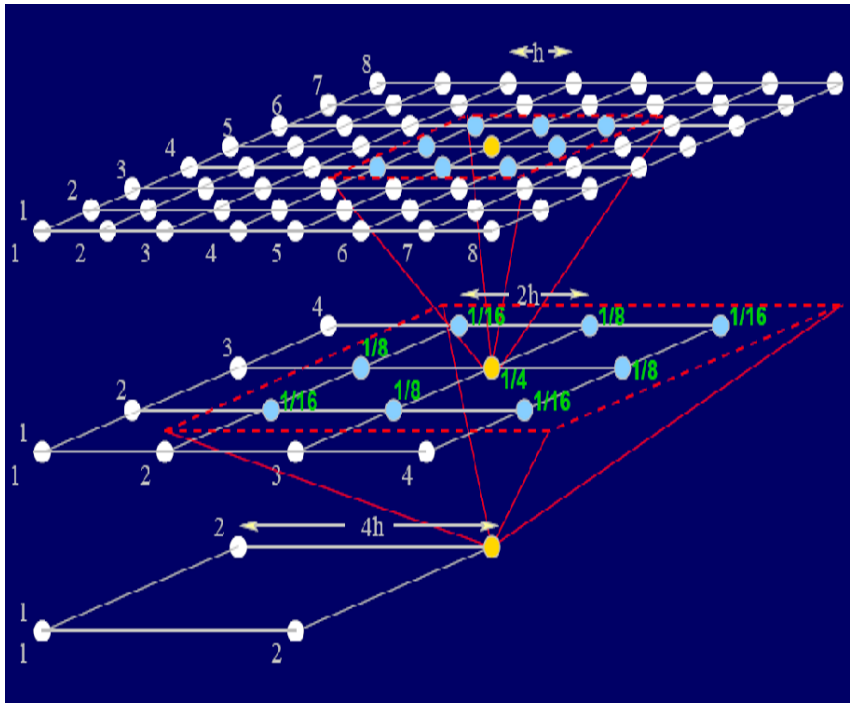

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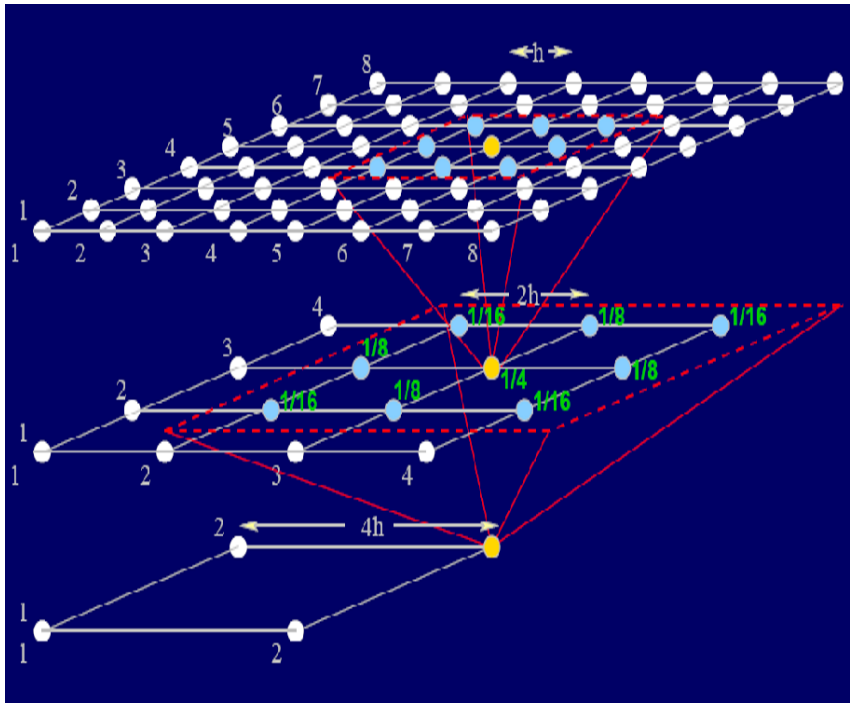

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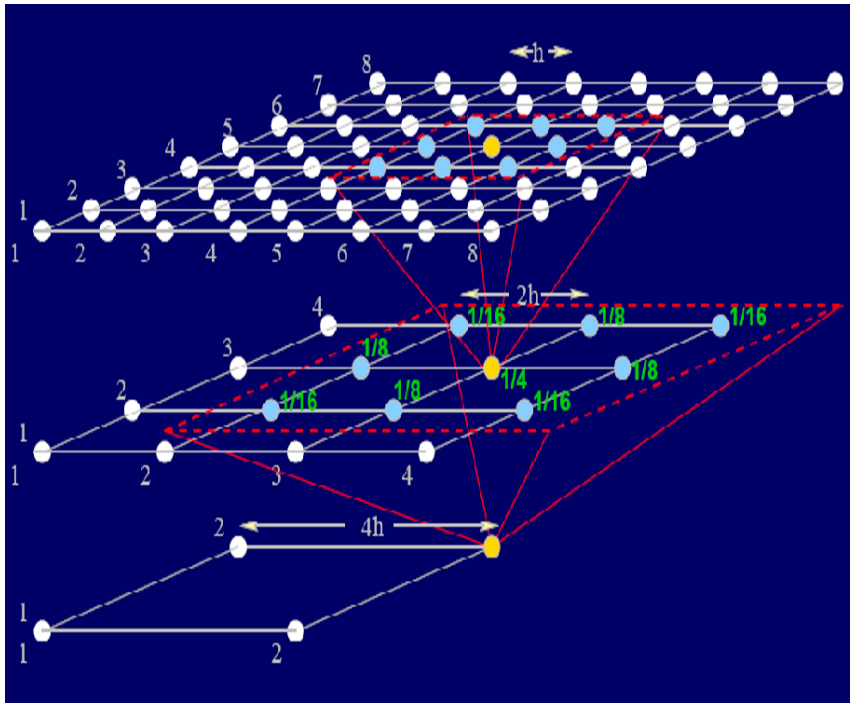

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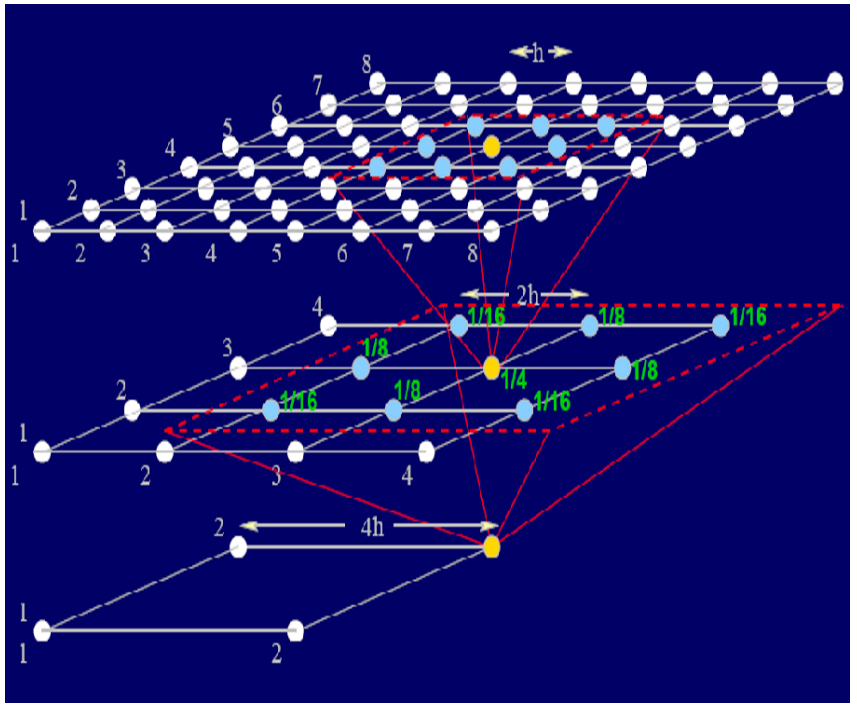

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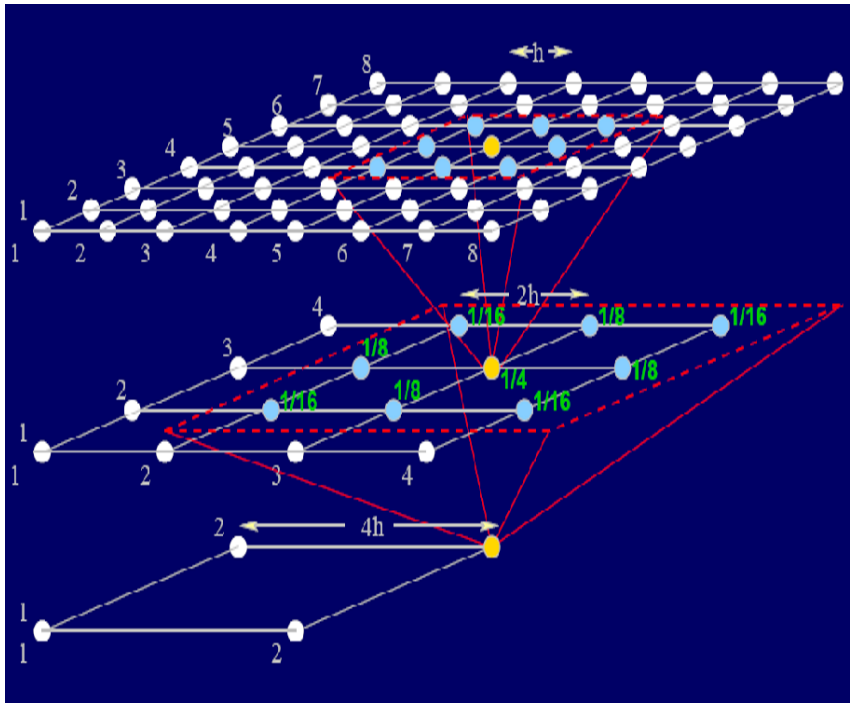

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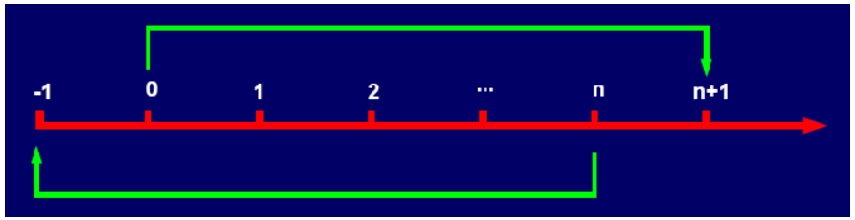

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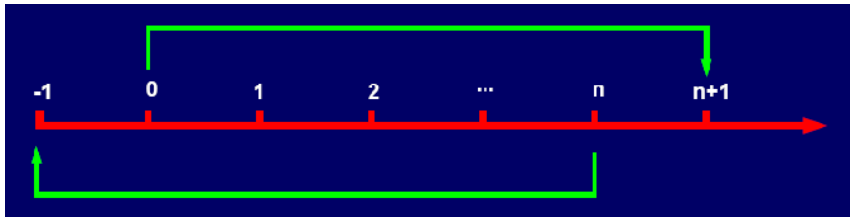

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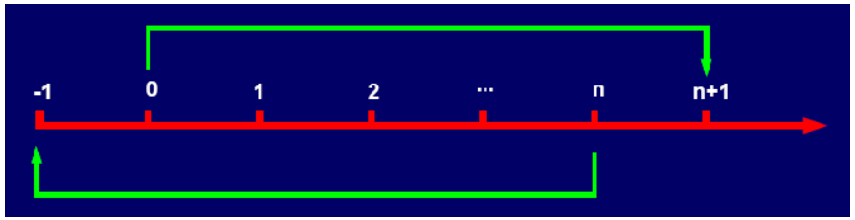

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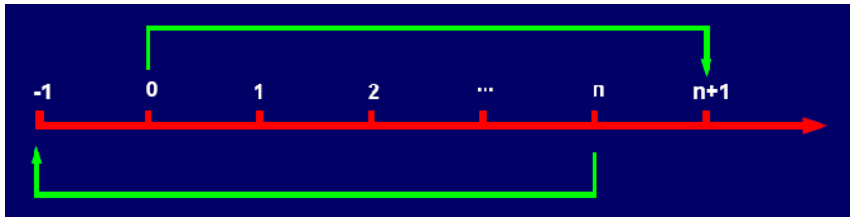

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  - Non-cyclic lateral conditions require the use of the multigrid-method for solving the Poisson-equation.

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- Surface boundary condition:
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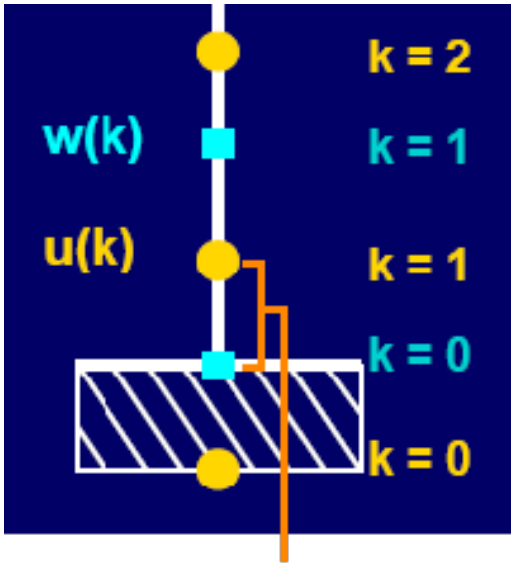

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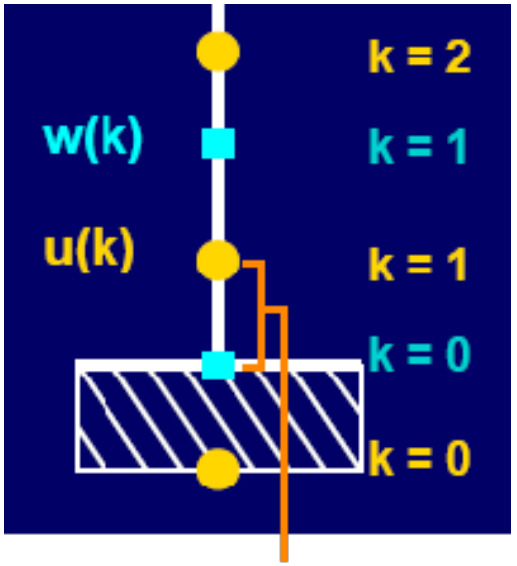

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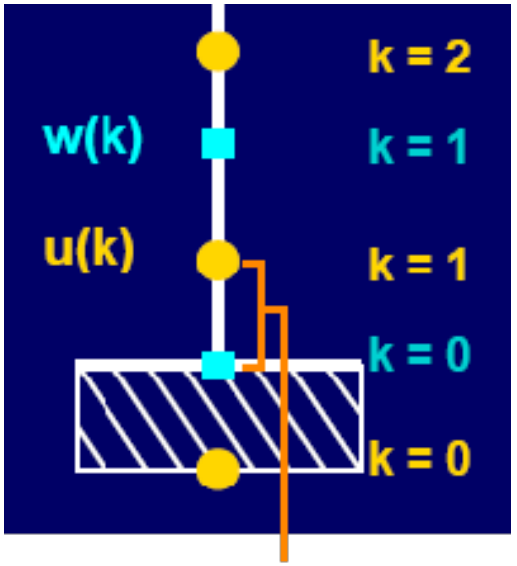

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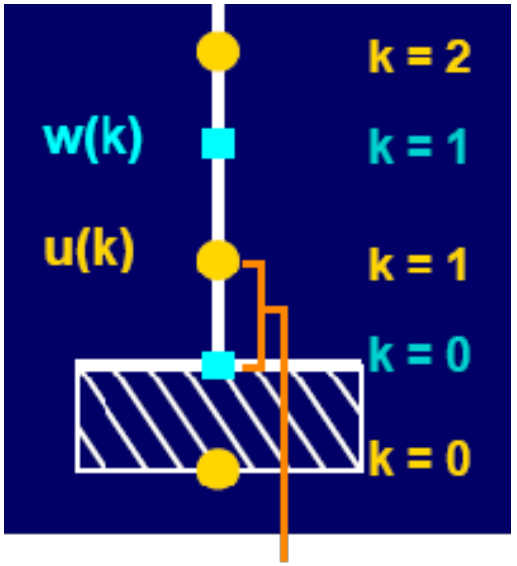

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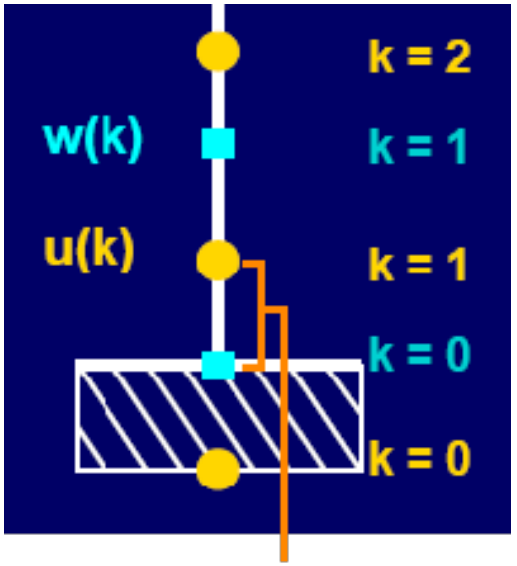

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$$\mathrm{Rif} = \frac{\frac{g}{\tilde{\theta}}\overline{w'\theta'_0}}{\overline{w'u'}\frac{\partial \overline{u}}{\partial z}}$$

Richardson flux number

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Under horizontally homogeneous initial conditions, random fluctuations have to be added in order to generate turbulence!