# Transport, chemistry and improved parallelization of the «pressure solver» in the regional atmospheric model MésoNH

**Jean-Pierre Pinty** (LA), **Christine Lac** (MF),
**Juan Escobar** (LA),
**Florian Visentin** (soon @ Polytech Montréal)
**Tomislav Maric** (now @ UW)
(under contract with the financial support of ANR SOLSTICE)
and other collaborators @ LA and MF

Work package 2.2.2

Final workshop SOLSTICE, June 2010

# Outlines:

- **New transport schemes:** Introduction of a PPM scheme for the 3D advection of the scalar fields and a family of WENO schemes for the 3D advection of the momentum

- **Chemical solver:** Introduction of a ½ implicit solver (Rosenbrock method) to integrate stiff chemical mechanisms

- **Improved parallelization of an elliptical solver:** Solve for $\Phi$ in GDIV($\rho \bullet \vec{\nabla}\Phi$)=F, where GDIV is the Generalized DIVergence operator, using FFT(x,y)-FFT$^{-1}$(x,y) and Tridiag(z) solver

# New transport schemes (1)

SCALAR **{S}**

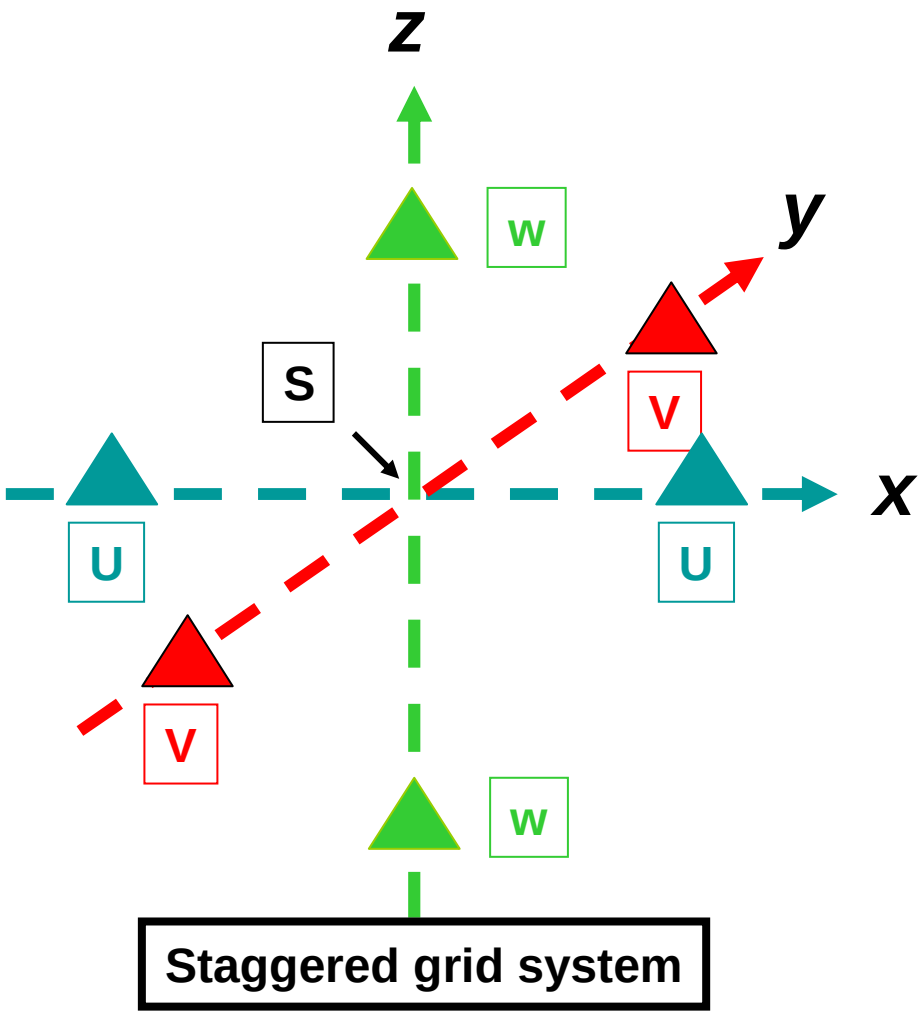
$$\frac{\partial \rho S}{\partial t} = \frac{\partial \rho S u}{\partial x} + \frac{\partial \rho S v}{\partial y} + \frac{\partial \rho S w}{\partial z}$$

MOMENTUM **{U, V, W}**

$$\frac{\partial \rho u}{\partial t} = \frac{\partial \rho u u}{\partial x} + \frac{\partial \rho u v}{\partial y} + \frac{\partial \rho u w}{\partial z}$$

$$\frac{\partial \rho v}{\partial t} = \frac{\partial \rho v u}{\partial x} + \frac{\partial \rho v v}{\partial y} + \frac{\partial \rho v w}{\partial z}$$

$$\frac{\partial \rho w}{\partial t} = \frac{\partial \rho w u}{\partial x} + \frac{\partial \rho w v}{\partial y} + \frac{\partial \rho w w}{\partial z}$$




**Momentum and Scalars are NOT colocalised ➔ ≠ numerical schemes**

# Advanced transport schemes (2) upstream conservative schemes

**Scheme for Scalar fields:** the **Piecewise Parabolic Method** (Woodward and Collela, JCP, 1984) is a Godunov scheme ➔ T. Maric

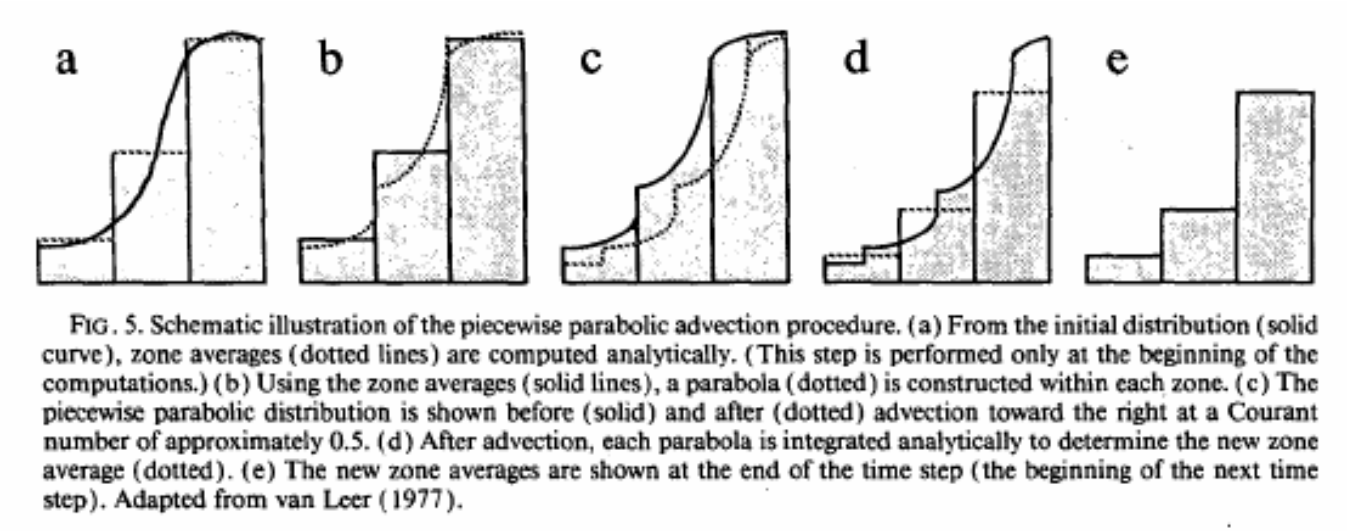



FIG. 5. Schematic illustration of the piecewise parabolic advection procedure. (a) From the initial distribution (solid curve), zone averages (dotted lines) are computed analytically. (This step is performed only at the beginning of the computations.) (b) Using the zone averages (solid lines), a parabola (dotted) is constructed within each zone. (c) The piecewise parabolic distribution is shown before (solid) and after (dotted) advection toward the right at a Courant number of approximately 0.5. (d) After advection, each parabola is integrated analytically to determine the new zone average (dotted). (e) The new zone averages are shown at the end of the time step (the beginning of the next time step). Adapted from van Leer (1977).

**Configuration:** wind components are located on the edge of each cell

**Advantages:** high accuracy, positive definiteness, monotonicity, stability up to CFL<1.0

# Advanced transport schemes (3) upstream conservative schemes

**Scheme for Momentum:** the **Weighted Essentially Non Oscillating** family of scheme (Liu, Osher, Chan, JCP, 1994) is TVD ➔ F. Visentin

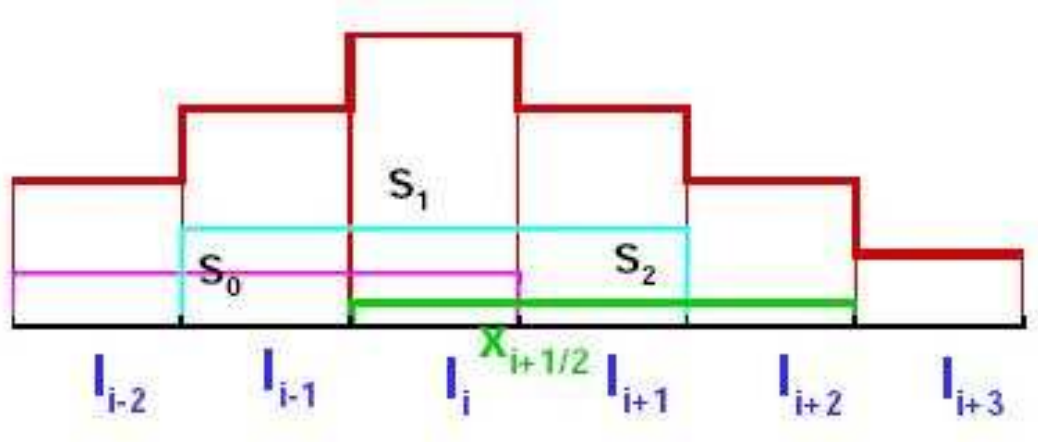



Illustration of **WENO5$^{th}$ order** : 3 stencils to estimate the advective fluxes, the weights are depending on the local smoothness of the field

**Configuration:** wind components and their tendencies are colocalized

**Advantages:** high accuracy, positive definiteness, monotonicity, stability up to CFL<1.

# Advanced transport schemes (4) upstream conservative schemes

**Temporal integration:** **Forward in Time** scheme

$$\frac{\partial \rho S}{\partial t} = \frac{(\rho S)^{t+\Delta t} - (\rho S)^{t}}{\Delta t}$$

… in place of the centered « leap-frog » scheme. OK for PPM and WENO1, WENO3 but unstable for WENO5.

➔ nSSP-RK scheme is required to integrate a WENO5$^{th}$ order scheme, e.g. 2 level-RK1 scheme (Wang and Spiteri, 2007):

$$(\rho S)^{t^*} = (\rho S)^{t} + 0.75 \times \Delta t \times \frac{\partial (\rho S)^{t}}{\partial t}$$

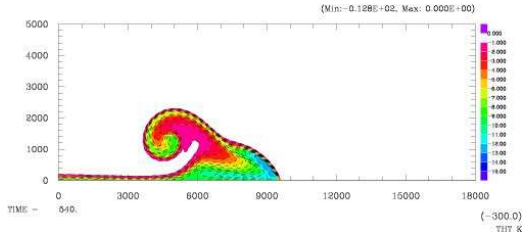
$$(\rho S)^{t+\Delta t} = (\rho S)^{t} + \Delta t \times \frac{\partial (\rho S)^{t^*}}{\partial t}$$

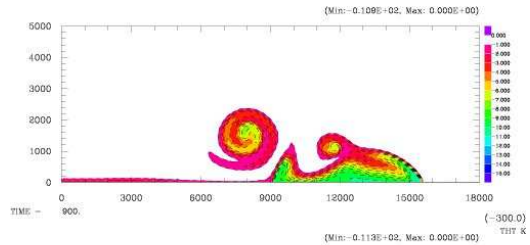
# Advanced transport schemes: « cold bubble » academic test case

Dx=Dz=50m, Dt=0.5 s, pert. -16.2K, Isentropic dry atmos.,
low diffusion 20Δ(u,w,Θ), Pr=1, **PPM for Θ**

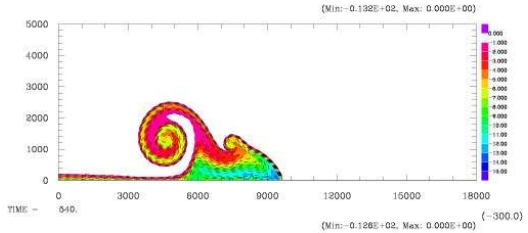
**Flow tracer is δΘ, $CFL_{max}$~ 0.5**

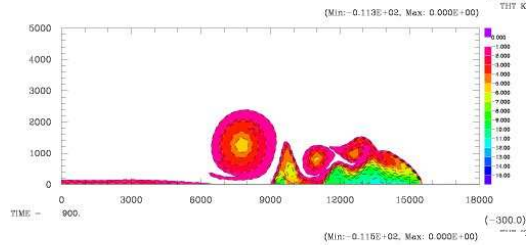
WENO1
FiT



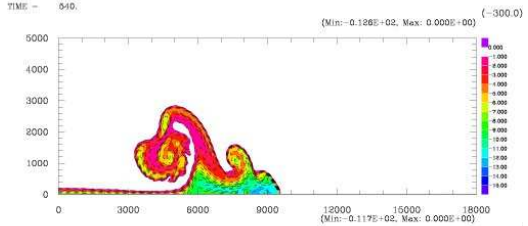


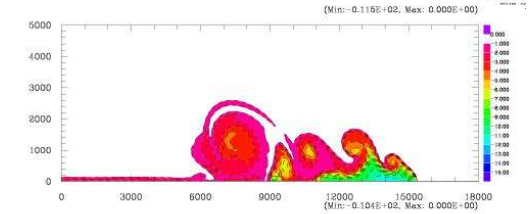
WENO3
FiT



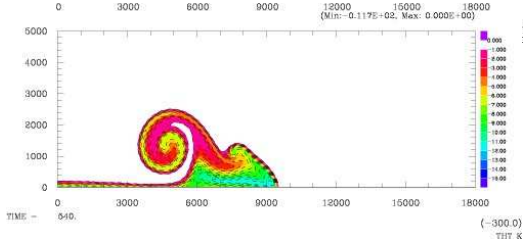


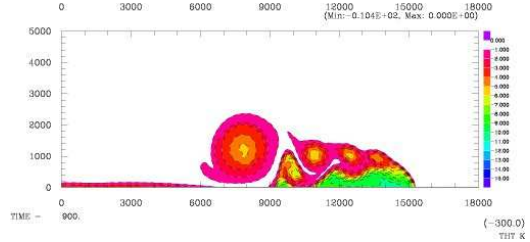
WENO5
FiT (unst.)





WENO5
nSSP-RK1

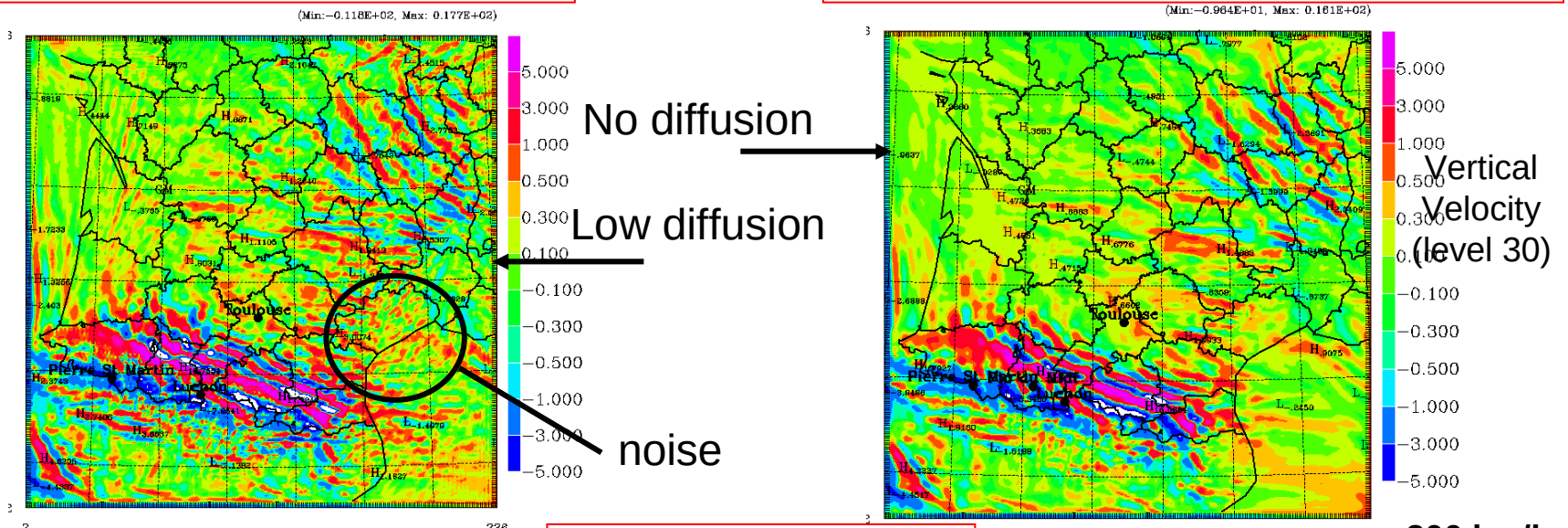


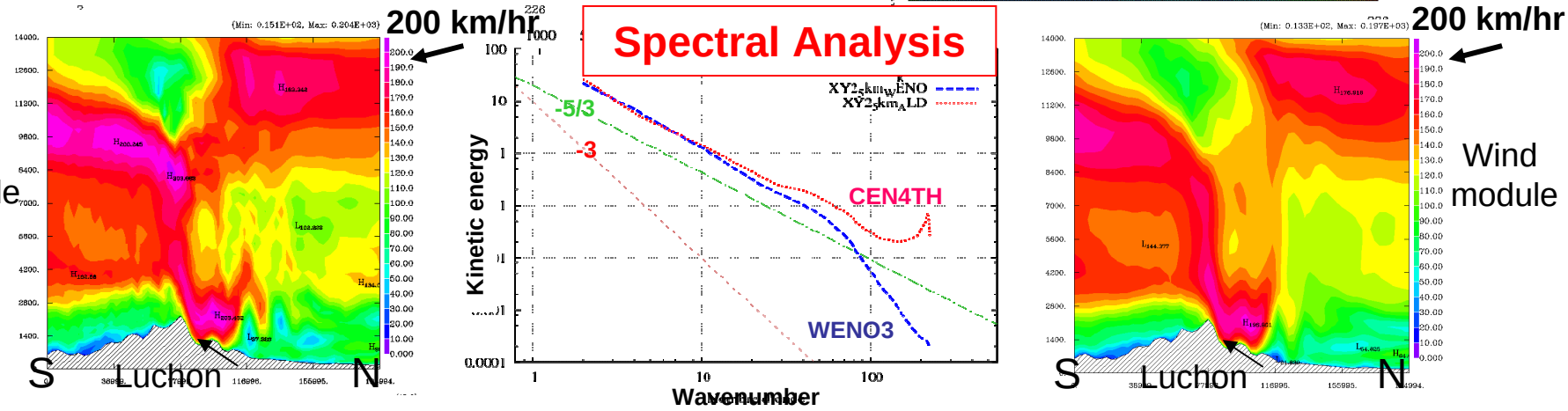


# Advanced transport schemes:
# « Xynthia » real test case

MESO-NH 2.5km, **5s**, **CEN4TH-LF**

MESO-NH 2.5km, **10s**, **WENO3-FIT**



# New scheme to integrate the gaseous-aqueous chemistry (1)

• Reactive system with *Nreact* ($k_\alpha$ photolytic rate or Arrhenius):

$$R_1 + R_2 + \cdots + R_{n_\alpha} \xrightarrow{k_\alpha} P_1 + P_2 + \cdots + P_{m_\alpha}$$

• Concentration equations $\mathbf{C=[C}_i\mathbf{]=\{}\boldsymbol{R+P\text{-}Fixed}\mathbf{\}}$ of prognostic species

$$\frac{\partial \rho \mathbf{C}}{\partial t} = -\nabla(\rho \mathbf{C} U) - \nabla \cdot \left(\rho \overline{\mathbf{C}' U'}\right) + \sum_{\alpha=1}^{Nreact} \sigma_{i\alpha} T_\alpha$$

**Eulerian transport**

**Turbulent transport**

**Chemical kinetics**

with

$$T_\alpha = k_\alpha \prod_{l=1}^{n_\alpha} [\mathbf{C}_l] \quad \text{and} \quad \sigma_{i\alpha} = \begin{cases} +1 & \text{when “i” is a product of the chem. reaction α} \\ -1 & \text{when “i” is a reactant of the chem. reaction α} \\ 0 & \text{otherwise} \end{cases}$$

# New scheme to integrate the gaseous-aqueous chemistry (2)

- Reactive mechanism with $\mathbf{C}^{\mathbf{gas}}$ and $\mathbf{C}^{\mathbf{aqu}}$ species linked by a **mass transfer $k_t$** term

$$\frac{\partial \mathbf{C}^{\mathbf{gas}}}{\partial t} = \cdots - L\,k_t\,\mathbf{C}^{\mathbf{gas}} + \frac{k_t}{RT\,H_{eff}}\mathbf{C}^{\mathbf{aqu}}$$

$$\frac{\partial \mathbf{C}^{\mathbf{aqu}}}{\partial t} = \cdots + L\,k_t\,\mathbf{C}^{\mathbf{gas}} - \frac{k_t}{RT\,H_{eff}}\mathbf{C}^{\mathbf{aqu}}$$

$L$ : cloud or rainwater content
$H_{eff}$ : effective Henry constant ($pH$, $T$)

**Aqueous phase**

- "pH" is a solution of a polynomial equation of degree 8
- Fast ionic reactivity for $\mathbf{C}^{\mathbf{aqu}}$ (oxidation of $S^{IV}$ → $S^{VI}$, …)
- Additional terms for $\mathbf{C}^{\mathbf{aqu}}$ due to droplet-drop conversion and rain sedimentation

**➔ very stiff chemical system requiring a stable and efficient method of integration**

# New scheme to integrate the gaseous-aqueous chemistry (3)

- **Rosenbrock solver**: a L-stable, iterative and conservative method with variable time step increment (error tolerance)

$$\frac{\partial \mathbf{C}}{\partial t} = \sum_{\alpha=1}^{Nreact} \sigma_{i\alpha} T_{\alpha} = \mathrm{F}(\mathbf{C}) \quad ===> \quad \mathbf{C}(t+\Delta t) = \mathbf{C}(t) + \sum_{i=1}^{s} c_i \mathbf{k_i}$$

$$\left(\mathrm{I} - \boldsymbol{\gamma}\Delta t \cdot \mathrm{F}'\right) \cdot \mathbf{k_i} = \Delta t \cdot \mathrm{F}\left(\mathbf{C}(t) + \sum_{j=1}^{i-1} \boldsymbol{\alpha}_{ij} \mathbf{k_j}\right) + \Delta t \cdot \mathrm{F}' \cdot \sum_{j=1}^{i-1} \boldsymbol{\gamma}_{ij} \mathbf{k_j}$$

- $\mathrm{F}'$ is the Jacobian matrix of the chemical system $\mathrm{F}$
- The coefficients $c_i$, $\boldsymbol{\gamma}$, $\boldsymbol{\gamma}_{ij}$, $\boldsymbol{\alpha}_{ij}$ are kept constant and given *a priori*
- Taking $\boldsymbol{\gamma}=\boldsymbol{\gamma}_{ij}=\mathbf{0}$, leads to an explicit Runge-Kutta scheme

Note: In MésoNH, $\mathrm{F}$ and $\mathrm{F}'$ are provided automatically by a preprocessor
The Rosenbrock algorithm is adapted from A. Sandu & R. Sander (MPI, Mainz)

➔ **The Rosenbrock method needs to invert a sparse matrix**

# New scheme to integrate the gaseous-aqueous chemistry (4)

- LU decomposition:

$$\left(\mathrm{I} - \gamma h \mathrm{F}'\right) \cdot \mathbf{k_i} = (\mathrm{LU}) \cdot \mathbf{k_i} = \mathbf{Z}$$

- "back-forward" substitutions:

$$\mathrm{L} \cdot \mathbf{Y} = \mathbf{Z} \quad (\text{stage } 1)$$

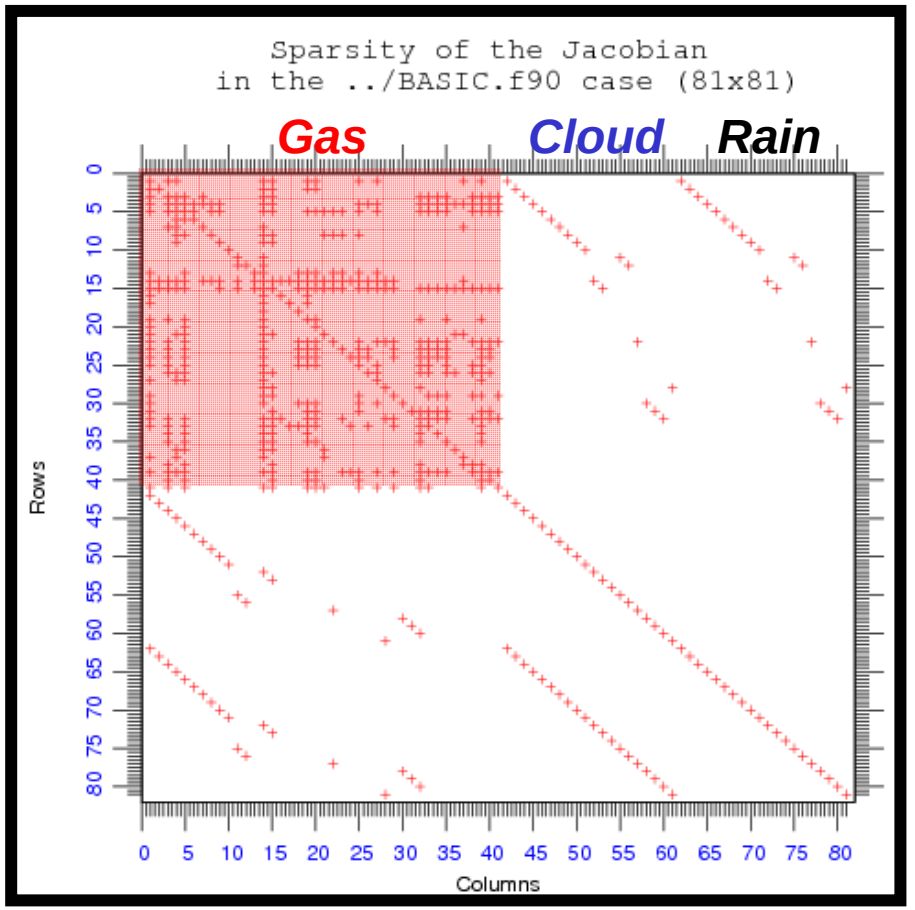
$$\mathrm{U} \cdot \mathbf{k_i} = \mathbf{Y} \quad (\text{stage } 2)$$

- **Sparse system algebra**:
  - Coding of indexes "Row" and "Col" of the non-zero matrix elements
  - Tagging of the "Diag" elements and of the 1st non-zero elements of each "Row"
  - Surprisingly, the LU and substitution algorithm is very short (about 40 lines of F90 code !!!)

- **Vectorization**: simultaneous treatment of several gridpoints → huge system to invert (with dimension up to Nspecies*Nx*Ny*Nz)

# Gaseous-aqueous chemistry: Idealized test case

- 2D tropical ideal. convective band off-shore Hawaii (180x60 grid points, $\Delta r$=50m, $\Delta t$=5s, $T_{end}$=50min)
- Kinematic flow circulation
- 41 **gas** + 2x20 **aqu** = **81 prognostic chemical species**
- **228 reactions**
- **Transport using PPM scheme**

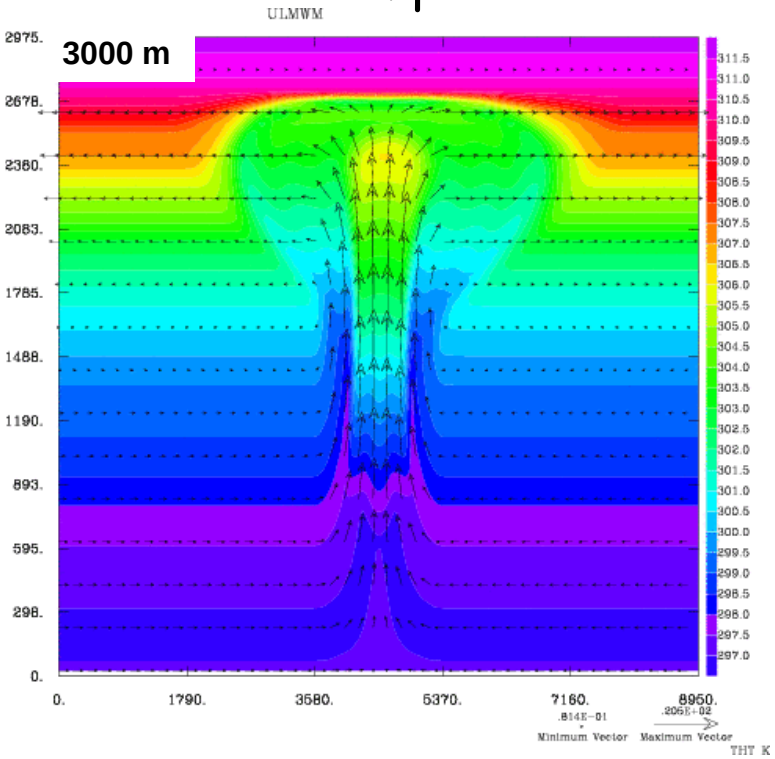


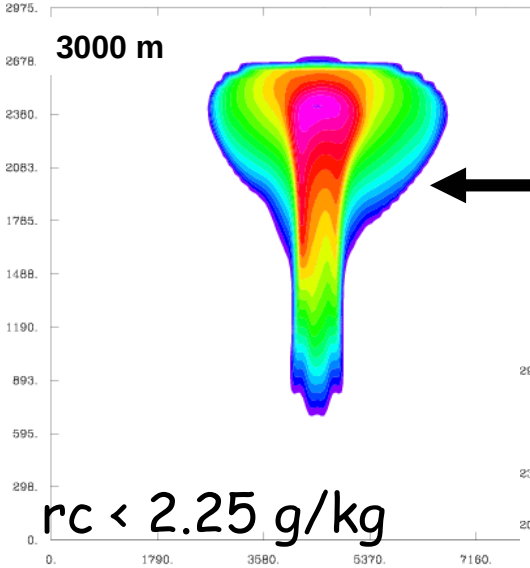

**794 non-zero elements**
(at each cloudy-rainy grid point)

**Each time step, the dimension of the chemical system to solve lies between**
180x60x41 = **442 800** grid points without cloud & rain
180x60x81 = **874 800** grid points are cloudy or rainy

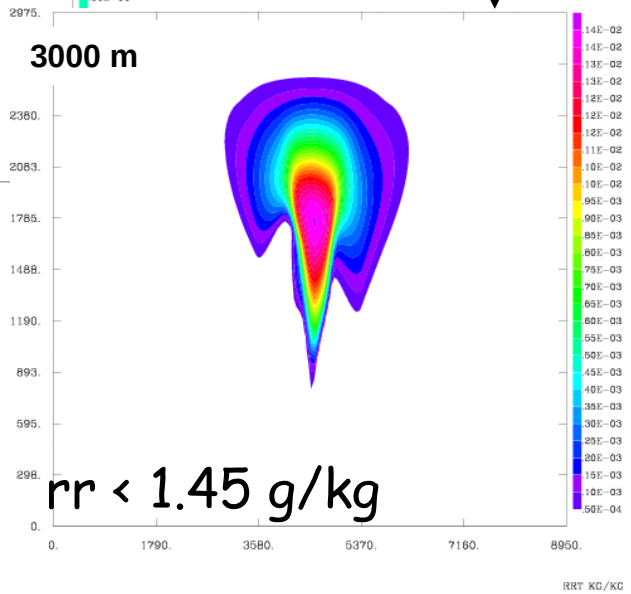
# Meteorological context
## at T=25mn

Potential Temperature
Wind components u et w



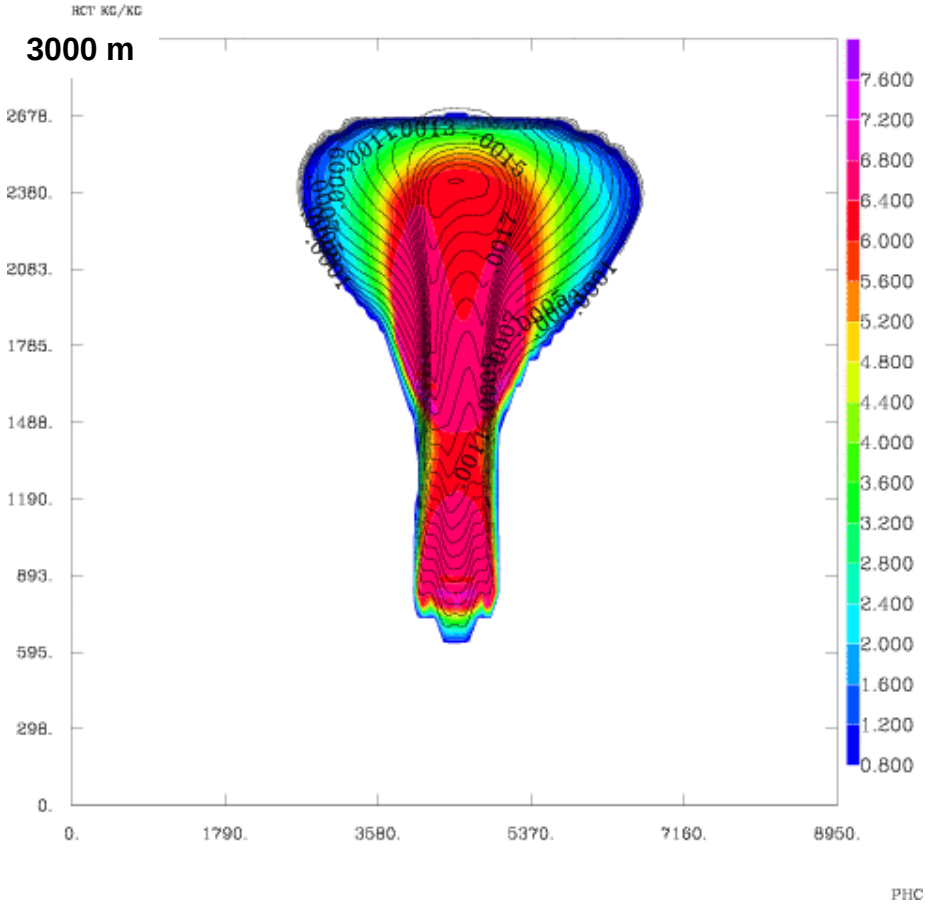




Water contents
Cloud and Rain

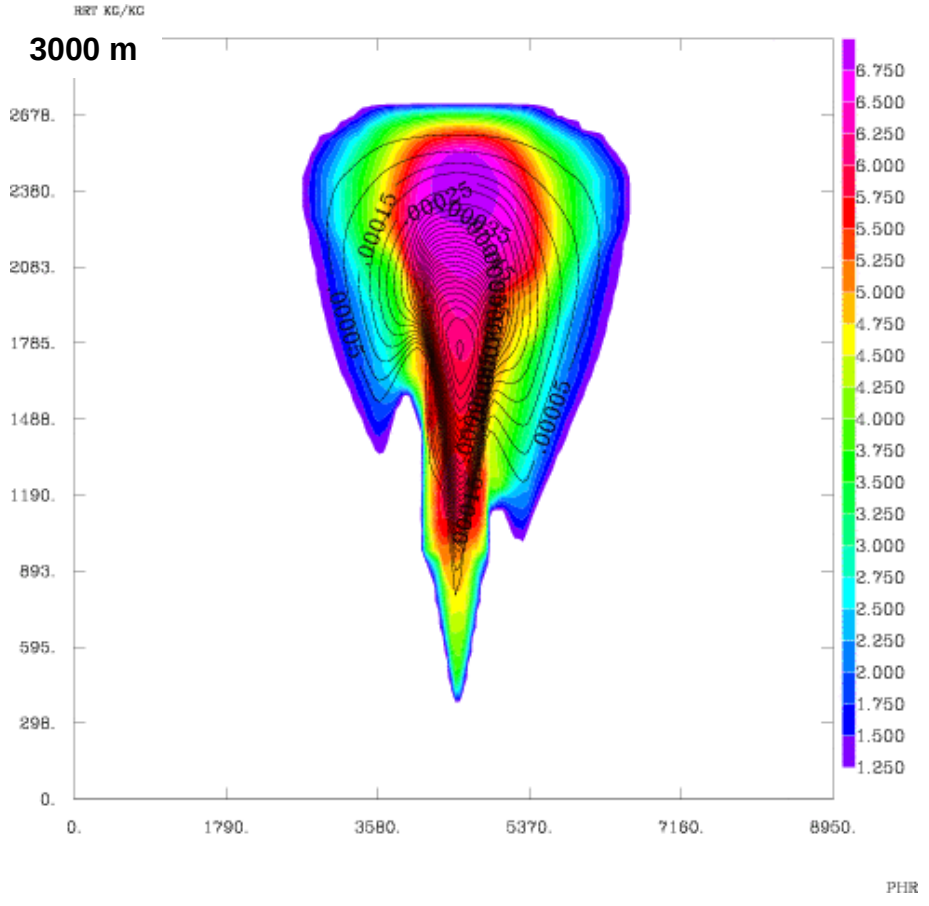


# pH calculation

## Cloud water




## Rain water



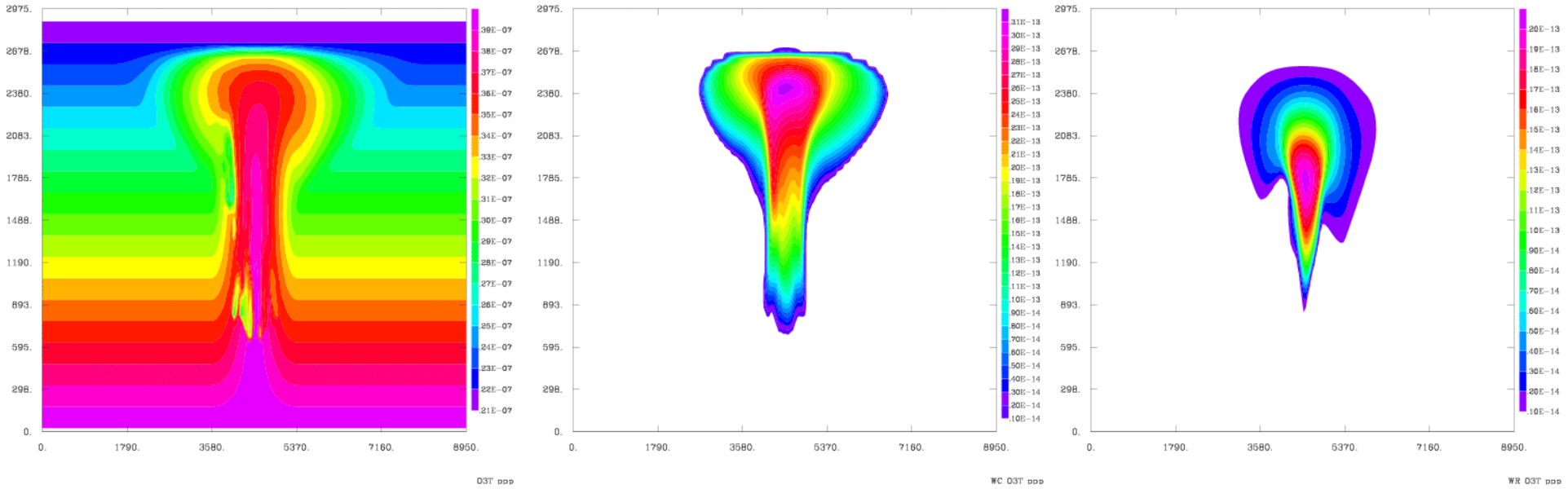
# Poorly soluble specy: $O_3$

Gaseous phase

Aqueous phase

Cloud

Rain




O3 < 3E-8 pp

WC_O3 < 3E-14 pp

WR_O3 < 2E-14 pp

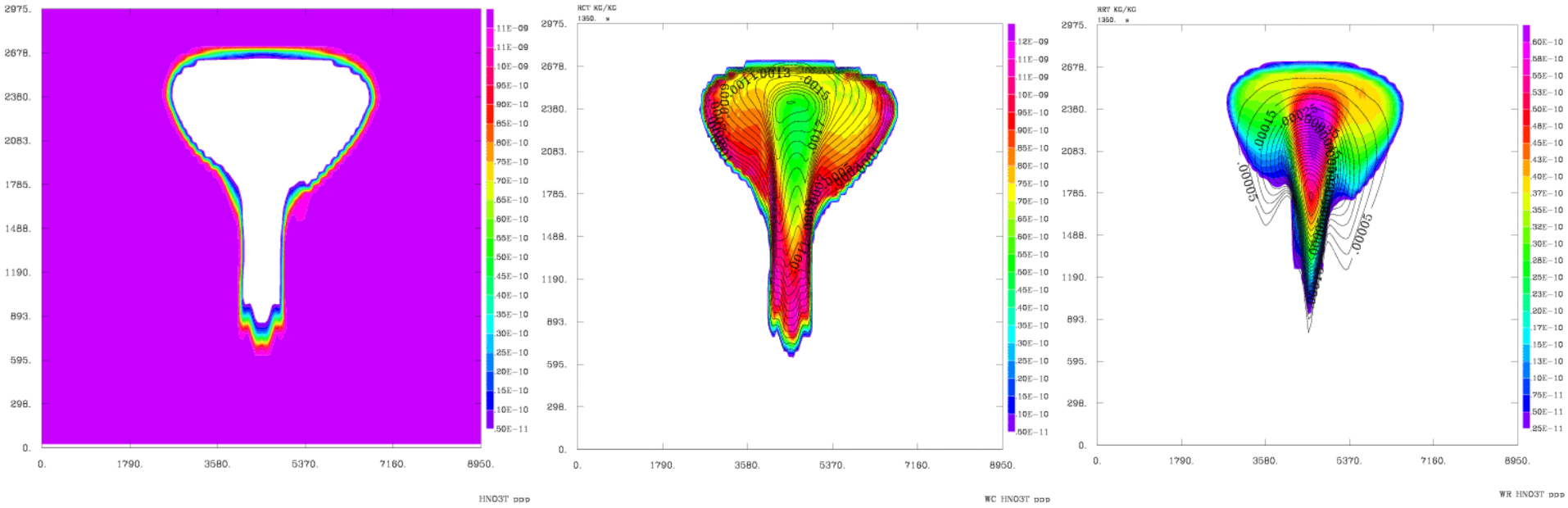
# Highly soluble specy: $HNO_3$

Gaseous phase

Aqueous phase

Cloud

Rain



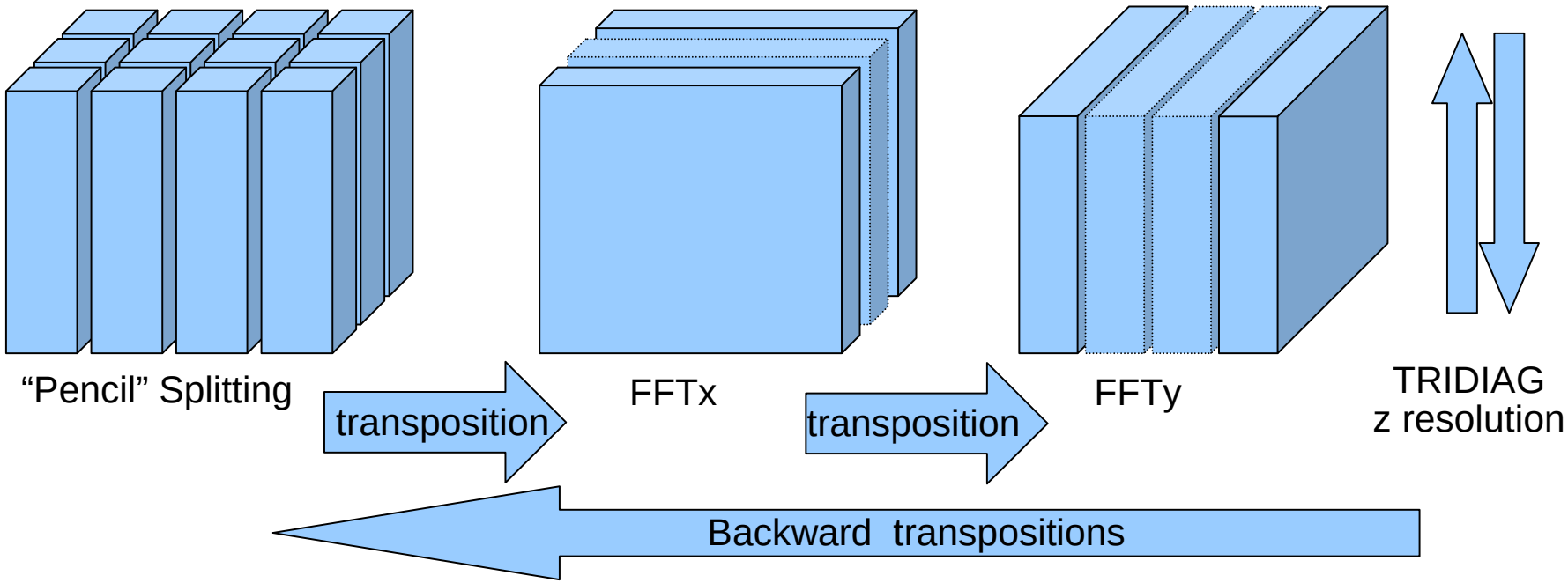

HNO3 < 5E-12 pp

WC_HNO3 < 1.2E-10 pp

WR_HNO3 < 6E-11 pp

# Extended parallelization of the elliptical solver of MesoNH (1)

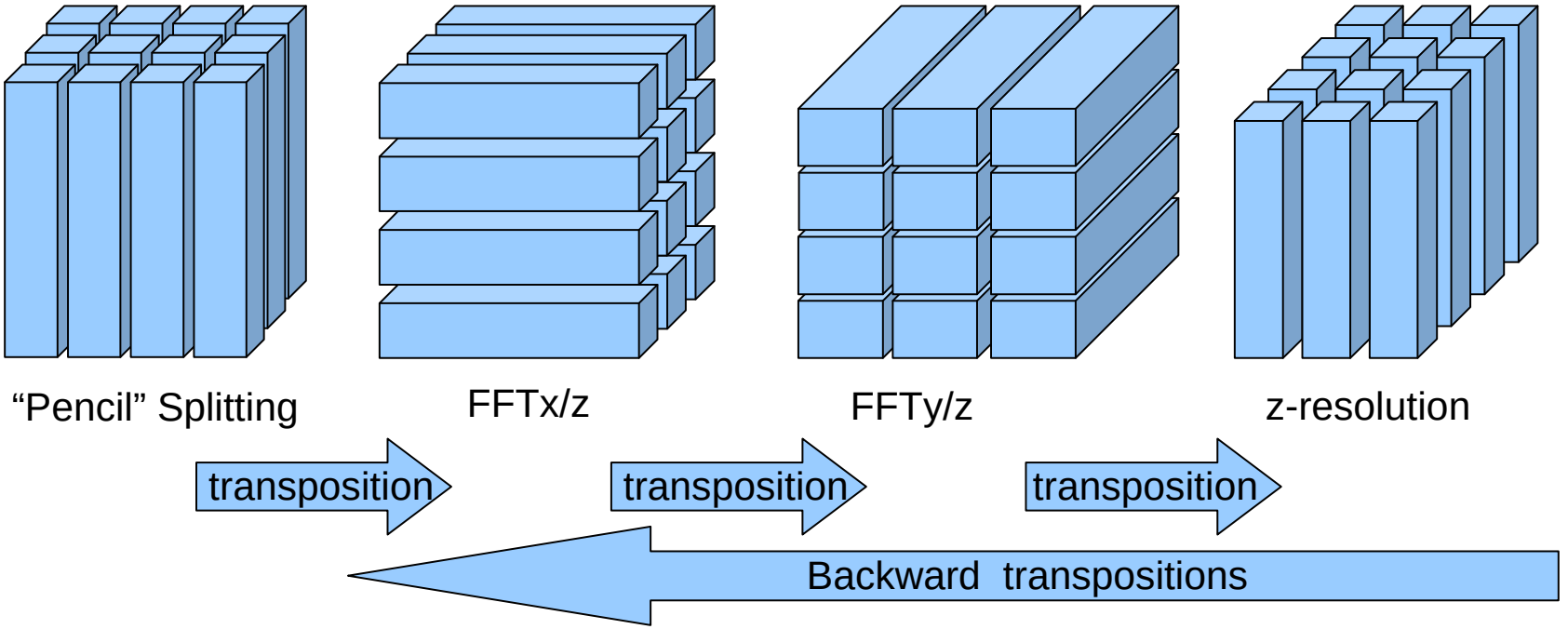
**Context:** Solving for $\Phi$ in GDIV($\rho \bullet \vec{\nabla}\Phi$)=F using FFTx,y transforms on Nx*Ny*Nz domain of simulation




➔ **LIMITATION: Nproc < Min(Nx, Ny)**
**with typically 128<Nx~Ny<1024 rows**

# Extended parallelization of the elliptical solver of MesoNH (2)

**Improvement:** Additional parallelization along the z-axis (work done by J. Escobar, LA)

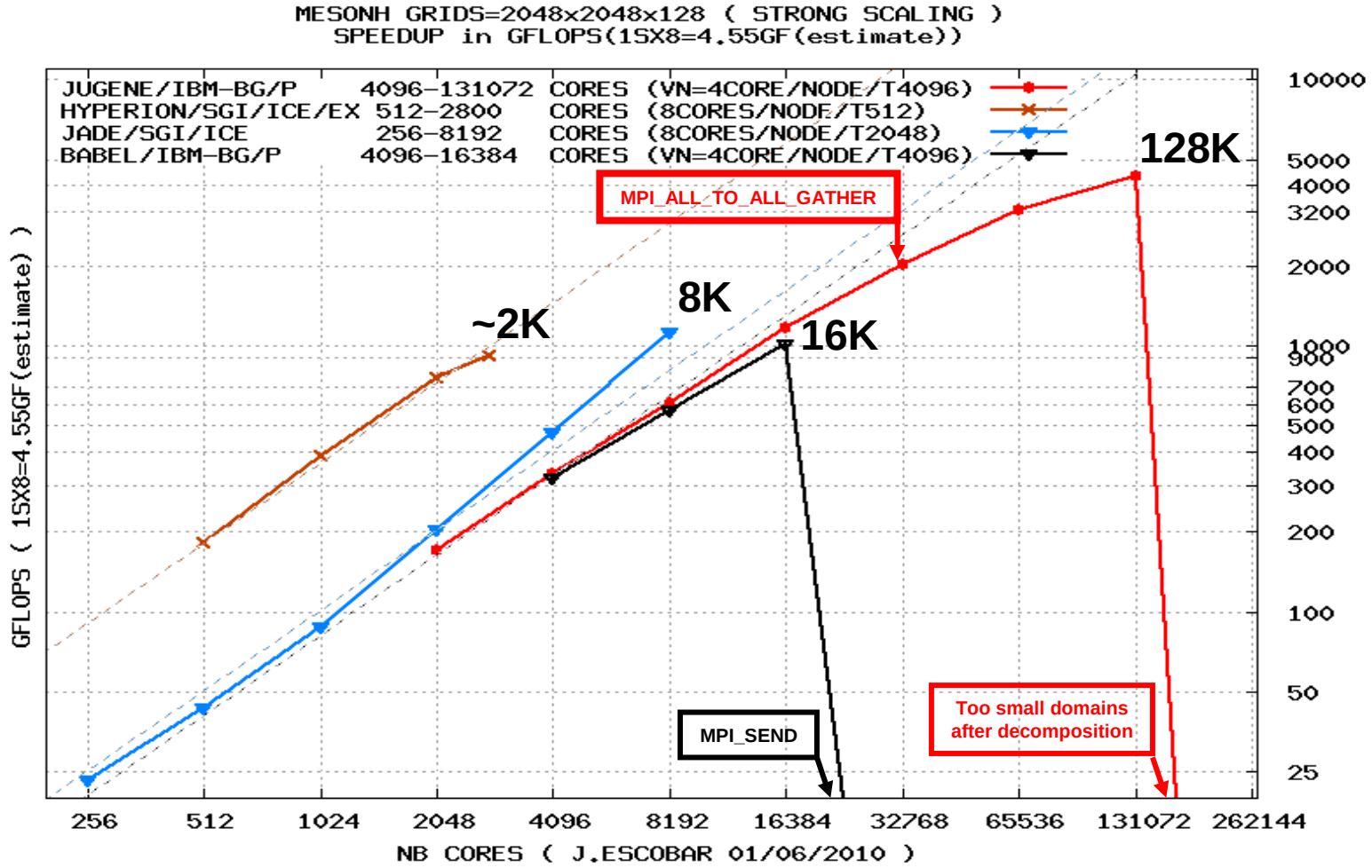



➔ **LIMITATION: Nproc < Min(Nx, Ny)xNz**

**128<Nx~Ny<1024 rows and 64<Nz<128 levels**

# Extended parallelization of the elliptical solver of MesoNH (3)

**Tests on MP machines:** performed by J. Escobar (LA)




Final workshop SOLSTICE, June 2010

# Extended parallelization of the elliptical solver of MesoNH (4)

**MesoNH top performance on MP machines**
after J. Escobar (LA)

PRACE special project in June 2010

IBM@Jülich : “JUGENE” BG/P 1 PETAFLOP

MESO-NH : 4 TERAFLOPS on 131 072 cores

# Conclusion

• **Transport schemes:** Parallelization of the WENO5 algorithm has to be done but the PPM+WENO3 parallelized implementation works successfully: increased time step & no additional diffusion term !

• **Chemical solver:** Extension to mixed-phase clouds is done. The vectorized Rosenbrock solver is working fine to integrate stiff chemical mechanisms (fast & accurate) !

• **Improved parallelization of an elliptical solver:** Enables to perform SIMD runs of MésoNH on MPM up to 128 Kcores !

➔ **Many thanks to ANR « SOLSTICE » for the support of these numerical and technical improvements of the MesoNH code**