# ETS Numerics – Quality Assessment / Verification

**WP09-ITM-IMP3-T2** $\Longrightarrow$ **WP10-ITM-IMP3-ACT1**

**Maintenance, continuing development,**
**(verification and validation) of the ETS**

## To discuss this week

1. **Staffing (**find volunteers**)**
   (a) "Users" – use existing ETS
   (b) "Developers" – extend ETS
2. **Verification procedure (**see below**)**
   (a) Basic numerical properties
   (b) Benchmarking vs. existing codes
3. **Time span (**July? 2010**)**

# Numerical properties

## Mandatory

1. Approximation
2. Accuracy
3. Convergence
4. Stability

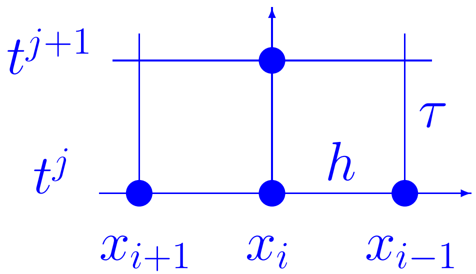
## Highly desirable

5. Conservation
6. Convection vs diffusion

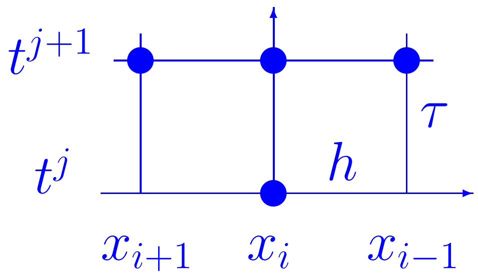
# **Approximation order** (finite differences)

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right) + S$$

**FTCS stencil**




**BTCS stencil**




$$\frac{\partial f(x,t)}{\partial t} = \frac{f_i^{j+1} - f_i^j}{\Delta t} + \frac{\partial^2 f}{\partial t^2}\Delta t + \ldots \implies \Delta f = \mathcal{O}(\Delta t), \quad \Delta t = t^{j+1} - t^j = \tau$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{f_{i+1}^j - 2f_i^j + f_{i-1}^j}{\Delta x^2} + \frac{\partial^3 f}{\partial x^3}\Delta x^2 + \ldots \implies \Delta f = \mathcal{O}(\Delta x^2), \quad \Delta x = x_{i+1} - x_i = h$$

The scheme has approximation error of order

$$\Delta f = \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2)$$

**Caveat:** For $\mathcal{N} = t/\Delta t$ time steps the error can accumulate and the **overall error** can be estimated as

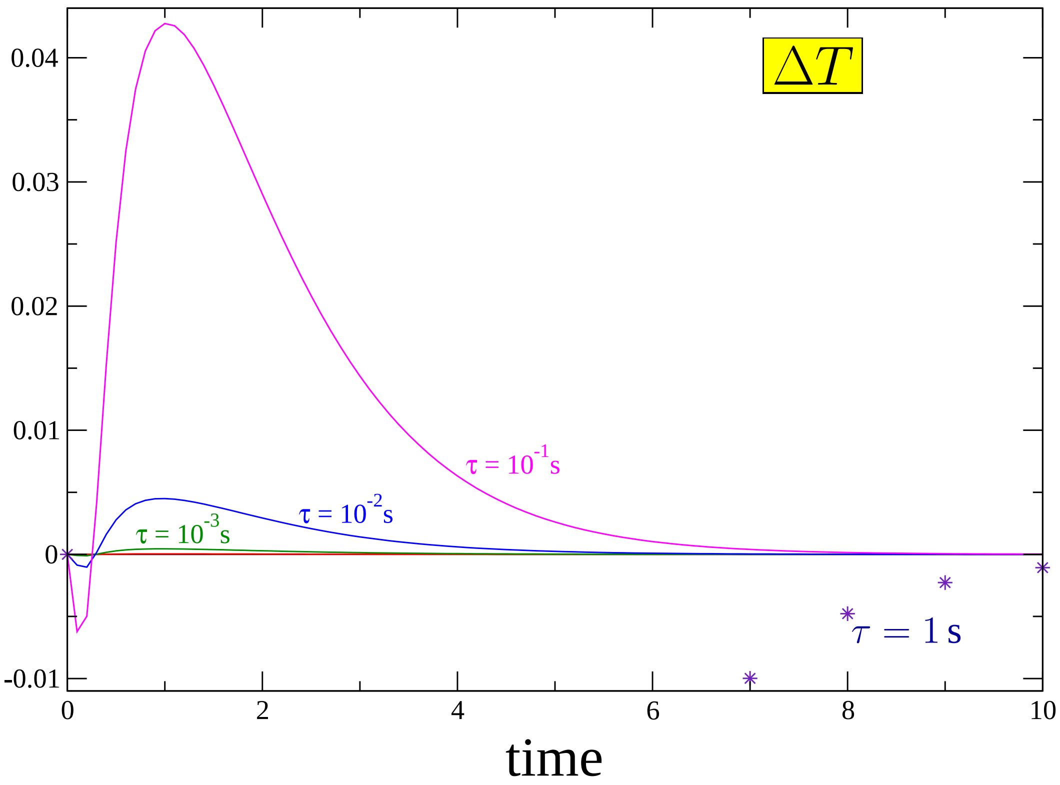
$$\mathcal{N} \times \Delta f = \frac{t}{\Delta t}\left[\mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2)\right] = \mathcal{O}(1)$$

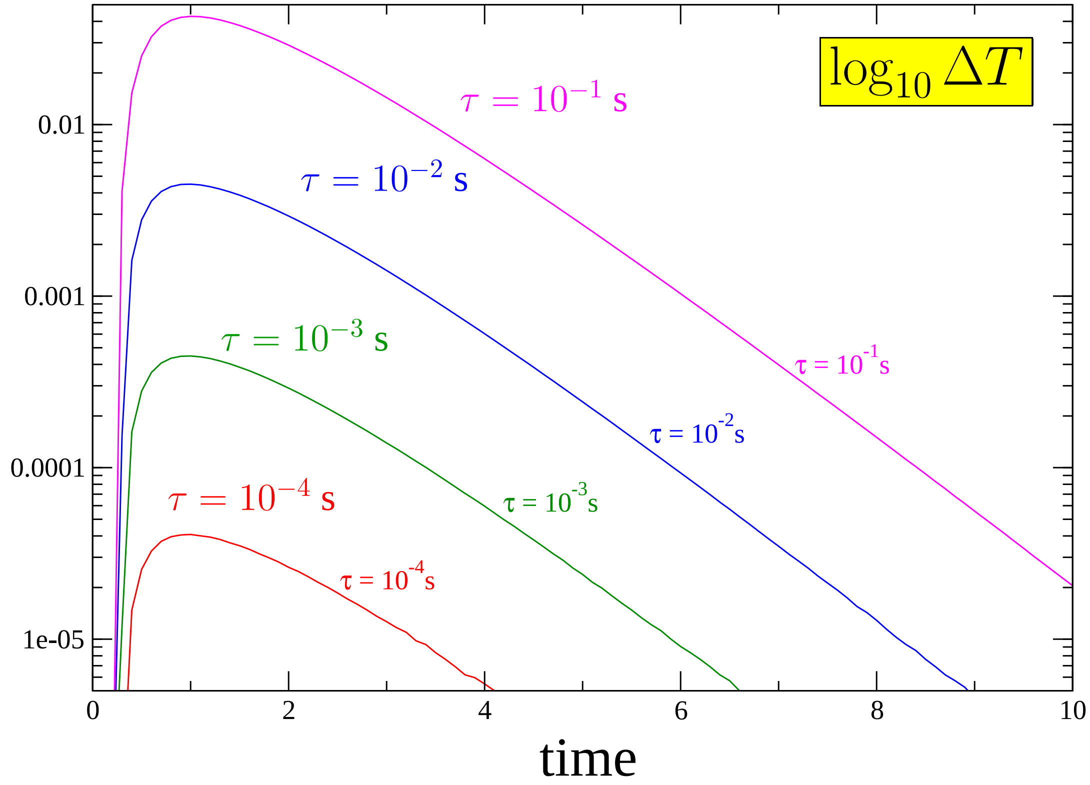
so that no **convergence** occurs.

# Numerical accuracy and convergence (examples)

$$\frac{3}{2}\left(V'\right)^{-5/3}\frac{\partial}{\partial t}\left[\left(V'\right)^{5/3} nT\right] = \frac{1}{V'}\frac{\partial}{\partial \rho}\left(V'\left\langle (\nabla\rho)^2\right\rangle \chi \frac{\partial T}{\partial \rho}\right) + P$$

## Time step dependence



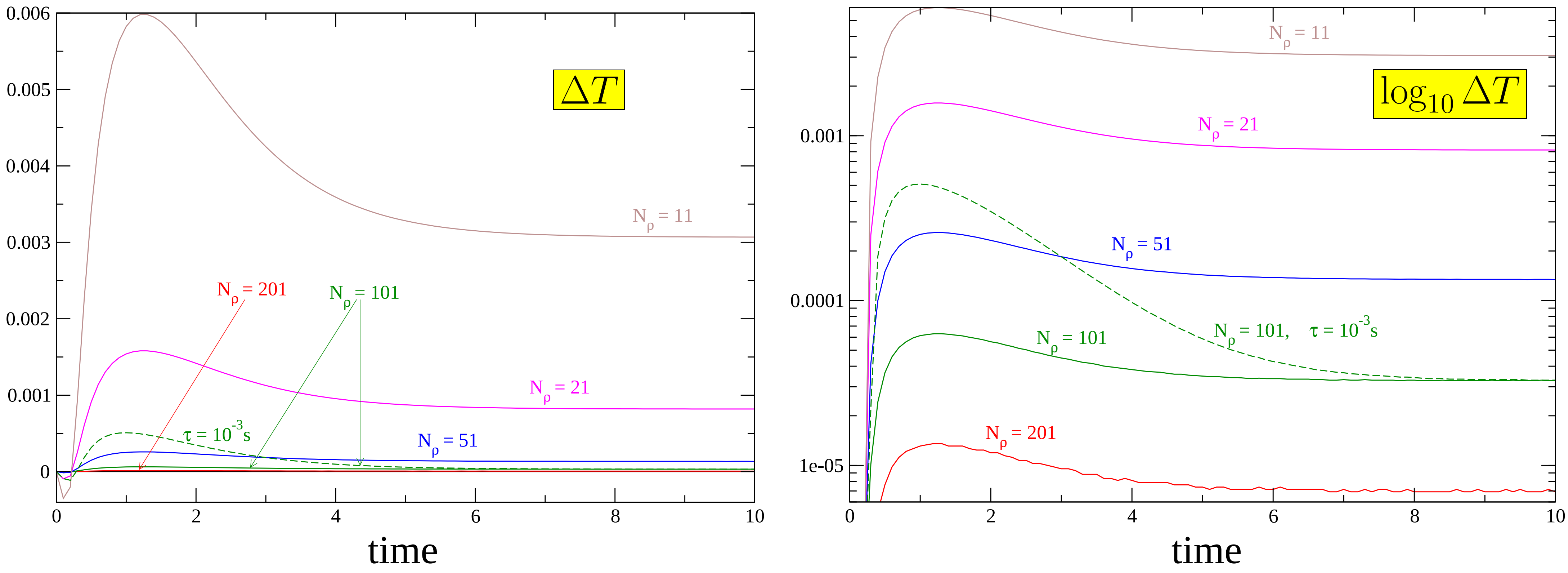




Maximum deviation as function of time for different time steps $\tau$. Reference run $\tau = 10^{-5}$s.

$\Delta T = \max_{\rho}\left(T - T_{ref}\right)$, $T_{ref} = T(\rho, t)$ calculated @ $\tau = 10^{-5}$s, $N_\rho = 501$

# Numerical accuracy and convergence (cont.)

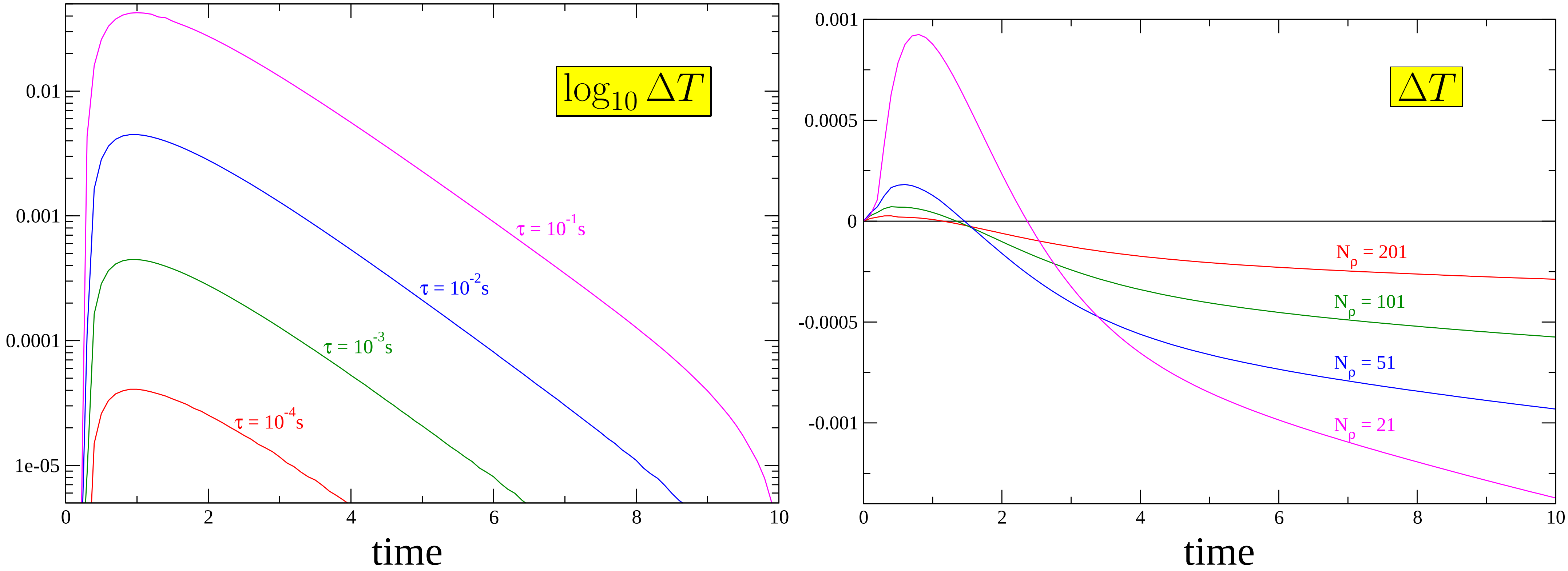
## Space step dependence




Maximum deviation as function of time for different grid sizes and $\tau = 10^{-5}$ s (dashed curve $\tau = 10^{-3}$ s).

# Numerical accuracy and convergence (cont.)

## Equilibrium (EMEQ) included



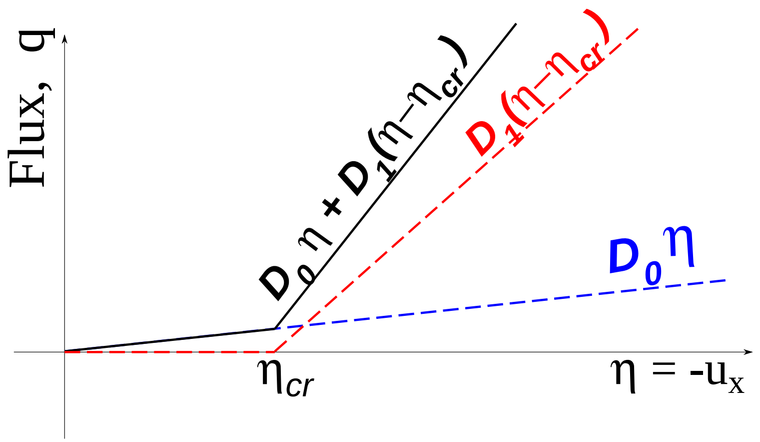

Maximum deviation as function of time for different grid sizes and $\tau = 10^{-5}$ s (dashed curve $\tau = 10^{-3}$ s).

# Stability

**Stiff diffusion equation**

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D_0\frac{\partial u}{\partial x} + D_{an}\left(\frac{\partial u}{\partial x} + \eta_{cr}\right)\right) + S$$

$$D_{an} = \begin{cases} D_1 \gg D_0, & \text{if } \left|\frac{\partial u}{\partial x}\right| > \eta_{cr} > 0, \\ 0, & \text{if } \left|\frac{\partial u}{\partial x}\right| < \eta_{cr}, \end{cases}$$




Straightforward approximation $\frac{\hat{u}_i - u_i}{\tau} = D_{i+1/2}\frac{\hat{u}_{i+1} - \hat{u}_i}{\Delta x^2} - D_{i-1/2}\frac{\hat{u}_i - \hat{u}_{i-1}}{\Delta x^2} + S_i$

requires a tiny time step $\tau \approx 10^{-5}s \leq 10^{-4}\,\frac{a^2}{D}.$

Possible scheme improvement (iterations with $0 \leq \sigma \leq 1$)

$$\frac{\hat{u}_i - u_i}{\tau} = \left(\sigma D_{i+1/2} + (1-\sigma)\hat{D}_{i+1/2}\right)\frac{\hat{u}_{i+1} - \hat{u}_i}{\Delta x^2} - \left(\sigma D_{i-1/2} + (1-\sigma)\hat{D}_{i-1/2}\right)\frac{\hat{u}_i - \hat{u}_{i-1}}{\Delta x^2} + S_i$$

# Conservation

**Exact conservation law:** $u_t = (Du_x)_x + S \quad \Rightarrow \quad \frac{\partial}{\partial t}\int_0^a u dV + \Gamma = \int_0^a S\, dV$

$$\frac{\hat{u}_i - u_i}{\tau} = D_{i+1/2}\frac{\hat{u}_{i+1} - \hat{u}_i}{\Delta x^2} - D_{i-1/2}\frac{\hat{u}_i - \hat{u}_{i-1}}{\Delta x^2} + S_i \qquad 0 \le i \le N$$

$$\frac{\hat{u}_0 - u_0}{\tau} = D_{1/2}\frac{\hat{u}_1 - \hat{u}_0}{\Delta x^2} + S_0 \qquad i = 0$$

$$\frac{\hat{u}_1 - u_1}{\tau} = D_{3/2}\frac{\hat{u}_2 - \hat{u}_1}{\Delta x^2} - D_{1/2}\frac{\hat{u}_1 - \hat{u}_0}{\Delta x^2} + S_1 \qquad i = 1$$

$+$

$$\frac{\hat{u}_2 - u_2}{\tau} = D_{5/2}\frac{\hat{u}_3 - \hat{u}_2}{\Delta x^2} - D_{3/2}\frac{\hat{u}_2 - \hat{u}_1}{\Delta x^2} + S_2 \qquad i = 2$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$\frac{\hat{u}_N - u_N}{\tau} = D_{N+1/2}\frac{\hat{u}_{N+1} - \hat{u}_N}{\Delta x^2} - D_{N-1/2}\frac{\hat{u}_N - \hat{u}_{N-1}}{\Delta x^2} + S_N \qquad i = N$$

**Numerical conservation law is exact for grid function**

$$\Delta x \sum_{i=0}^{N} \frac{\hat{u}_i - u_i}{\tau} = D_{N+1/2}\frac{\hat{u}_{N+1} - \hat{u}_N}{\Delta x} + \Delta x \sum_{i=0}^{N} S_i \quad \Rightarrow \quad \Gamma = -D_{N+1/2}\frac{\hat{u}_{N+1} - \hat{u}_N}{\Delta x}, \qquad S = \Delta x \sum_{i=0}^{N} S_i$$

# Conservation (cont.)

**Integral conservation law:**

$$\frac{\partial}{\partial t}\int_0^a u\,dV + \Gamma\Big|_a = \int_0^a S\,dV$$

**Numerical conservation law:**

$$\Delta x \sum_{i=0}^{N} \frac{\hat{u}_i - u_i}{\tau} = D_{N+1/2}\frac{\hat{u}_{N+1} - \hat{u}_N}{\Delta x} + \Delta x \sum_{i=0}^{N} S_i$$

- **Both conservation laws are exact.**
- **Existence of a numerical conservation ensures that some basic physics constraints are fulfilled.**
- **Convergence does not ensure that** $\Longrightarrow$ **Conservation is highly desirable**

**However, a form of numerical conservation law should be conforming with a numerical scheme.**

$\Rightarrow$ Change of numerics implies a change of the conservation law.
$\Rightarrow$ Not every numerical approximation possess a conservation property.
$\Rightarrow$ Non-conserving methods should not be used in ETS.
$\Rightarrow$ Conservation is not a consequence of approximation because the total error can be large enough.
$\Rightarrow$ Cross-process conservation laws have to be included.

**Examples of significance:**

Electron-ion equipartition
Particle conservation for impurities
Volt-second consumption

# Convective terms

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x} - Vu\right) + S$$

**The first-order upwind scheme**

$$\frac{\hat{u}_i - u_i}{\tau} = D_{i+1/2}\frac{\hat{u}_{i+1} - \hat{u}_i}{\Delta x^2} - D_{i-1/2}\frac{\hat{u}_i - \hat{u}_{i-1}}{\Delta x^2} - \min(V_{i+1/2}, 0)\frac{u_{i+1} - u_i}{\Delta x} - \max(V_{i-1/2}, 0)\frac{u_i - u_{i-1}}{\Delta x} + S_i$$

$= 0, \;\text{if}\; V_{i+1/2} > 0$ $\qquad$ $= 0, \;\text{if}\; V_{i-1/2} < 0$

**is stable but non-conservative.**

**The simple scheme**

$$\frac{\hat{u}_i - u_i}{\tau} = D_{i+1/2}\frac{\hat{u}_{i+1} - \hat{u}_i}{\Delta x^2} - D_{i-1/2}\frac{\hat{u}_i - \hat{u}_{i-1}}{\Delta x^2} - \frac{V_{i+1/2}u_{i+1/2} - V_{i-1/2}u_{i-1/2}}{\Delta x} + S_i$$

**is conservative but can become unstable.**

**In transport modelling convection is usually small.**

$\Longrightarrow$ **Problems can arise if** $V \geq D/a$

# V&V proposals for IMP3

## Users

1. Perform accuracy tests for each ETS solver.
   (a) Simple cases (including non-smooth, non-continuous coefficients).
   (b) Manufactured solutions.
   (c) Select the reference time and space steps $\{\Delta t, \Delta x\}$ for further studies.
2. Perform series of runs on conservation property.
3. Convection vs. diffusion.
4. Benchmarking: Run the test cases with ASTRA, JETTO, CRONOS.
5. Documentation for pp. 1 – 4 by July 2010.

$\Longrightarrow$ Validation procedure.

## Developers

1. Extend existing solver to include stiff transport.
2. Add more solvers (CRONOS, finite elements, . . . )

start_time_loop

READ_INPUT

start_iteration_loop

EQUILIBRIUM $\longrightarrow$ Internal iterations: Exit if $(\max \Delta_E < 10^{-5})$

SOURCE

TRANSPORT

CONVERGENCE_CHECK $\longrightarrow$ $\max \Delta_I < 10^{-4}$ ?

end_iteration_loop

CONVERGENCE_CHECK $\longrightarrow$ $\max \Delta_T < 10^{-3}$ ?

TIME_ADVANCE t=t+Δt, ...

end_time_loop

- Optimize the procedure
- Automated time step