Advances in Domain Decomposition Method techniques.

por Mario Storti, Norberto Nigro and Rodrigo Paz

Centro Internacional de Métodos Numéricos

en Ingeniería - CIMEC

INTEC, (CONICET-UNL), Santa Fe, Argentina

`<{mstorti,jdelia, rodrigop}@intec.unl.edu.ar>`

`http://www.cimec.com.ar`

`http://venus.ceride.gov.ar`

`(document-version "conf-0.0.1")`

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Outline of presentation

- **During last years, CFD group at CIMEC (Centro Internacional de Métodos Computacionales en Ingeniería, Santa Fe, INTEC-CONICET-UNL), develops a multi-physics, parallel, open-source CFD program called PETSc-FEM (`http://www.cimec.org.ar/petscfem`). We will present here an introduction to PETSc-FEM, its philosophy and recent developments.**
- **A technique to introduce first absorbing absorbing boundary conditions for advective-diffusive problems is presented. It allows to impose absorbing boundary conditions in situations where the number of incoming/outgoing characteristics is variable in space and time. We will see that this finally leads to using Lagrange Multipliers and penalization technique, which in turn require more robust iterative methods.**
- **The Interface Strip Preconditioner for Domain Decomposition Methods is presented. It improves convergence specially for badly conditioned problems.**

Introduction to PETSc-FEM

Until 1996 approx. CFD computations were carried with *good old* procedural Fortran programming. Then we decided to migrate our code and FEM know-how to more *“advanced programming”* techniques,

- **Parallel computing.**
- **Object Oriented Programming.**
- **Multi-physics.**
- **Scripting via extension languages (this feature added later, work is in progress).**

Parallel computing in PETSc-FEM

- **Experiences with parallel computing in CFD in CIMEC started in 1995 with a test code written in Fortran using MPI (Message Passing Interface), with two Digital-Alpha processors and Fast Ethernet (100 Mb/s). The program solved the compressible Euler equations with an explicit scheme.**
- **PETSc-FEM uses PETSc/MPI in C++. PETSc is the Portable, Extensible Toolkit for Scientific Computation (PETSc), a set of libraries and data structures to solve PDE's system of equations on HPC computers. PETSc was developed at the Argonne National Laboratory (ANL) by Satish Balay, William Gropp and others. `http://www.mcs.anl.gov/petsc/`. PETSc, while it is written in C, uses the OOP (Object Oriented Programming paradigm). Uses MPI for the low-level parallel communications.**

Parallel computing in PETSc-FEM (cont.)

- **PETSc-FEM implements the core Finite Element library in charge of assembly element matrices and residuals in parallel. This matrices and residuals are PETSc objects, and systems are solved with the PETSc library.**
- **Also implemented a new Domain Decomposition Method solver and a preconditioner (to be described later in this talk).**
- **PETSc-FEM runs on cluster of PC's using MPI (Beowulf clusters).**

Object Oriented Programming in PETSc-FEM

- **OOP is a programming paradigm that focus on the idea behind object-oriented programming is that a computer program is composed of a collection of individual units, or objects, as opposed to a traditional view in which a program is a list of instructions to the computer. Each object is capable of receiving messages, processing data, and sending messages to other objects. Object-oriented gives more flexibility and increases code reusability.**
- **C++ is a programming language based on C, that supports object-oriented programming while accepting also the procedural programming paradigm.**

Object Oriented Programming in PETSc-FEM (cont.)

The key idea behind OOP is PETSc-FEM is that large sets of data like nodes and elements (atoms) with the same characteristics are grouped in *`Atomsets`* (*vectors* or *arrays* of atoms). Atomsets provide the following items

- **Degrees of freedom (unknown, varying fields).**
- **Spatial data (known, constant fields).**
- **Links to other atoms in this Atomset or another. (e.g. FEM connectivity).**
- **Restrictions (e.g. boundary conditions)**
- **Functions that map the unknowns in a given atom (or its linked atoms) to residual or matrices. (The *“element routine”*).**

Object Oriented Programming in PETSc-FEM (cont.)

Some examples,

- **In finite elements we have nodes and elements as atoms. Nodes have unknown fields and also known fields (constant data). Node coordinates are simply a constant data field.**
- **In cell-centered finite volumes and panel methods (BEM) nodes have the coordinates constant fields, but unknowns reside in the cells. Also FEM has sometimes unknown fields in elements, for instance internal pressure nodes in BB-*a priori* stable interpolation families for incompressible flow.**
- **In applications with moving boundaries (e.g. ALE) coordinates are an unknown field. There are two FEM problems: the physical problem (for which coordinates are a constant field) and the mesh-moving pseudo-elastic problem (for which node coordinates are an unknown field).**

Object Oriented Programming in PETSc-FEM (cont.)

- **Fields can be added at the user-level, mapping functions operate on their specific fields, ignoring additional fields. (e.g. Navier-Stokes for fluid-dynamics with coupled transport on scalars).**
- **Several finite element problems may coexist in the same run, for instance the fluid problem and the mesh-moving one when dealing with moving domains (ALE).**

Object Oriented Programming in PETSc-FEM (cont.)

Elemset class hierarchy

- **Functions that map element states to residuals (and matrices) belong to the `Elemset` class. They represent the physics of each problem.**
- **Specialized mapping functions can share code with more general ones by *“class derivation”*. This originates an Elemset class tree.**
- **In this respect, the most paradigmatic case is the *advective-diffusive module*. A mapping function for generic advective-diffusive problems with the SUPG formulation has been implemented. Physical problems as gas dynamics, shallow water (1D and 2D), linear advection, Burgers eqs., share this. Each physical problem is added by writing a *“flux function class”*. This is an abstraction of the mathematical relation $U \to \mathcal{F}_c(U), \mathcal{F}_d(U)$, where U is the fluid state and $\mathcal{F}_{c,d}$ are the convective and diffusive fluxes.**
- **Flux function objects are shared between different stabilization schemes (e.g. FEM+SUPG, FVM) or absorbing boundary conditions.**

Physical properties

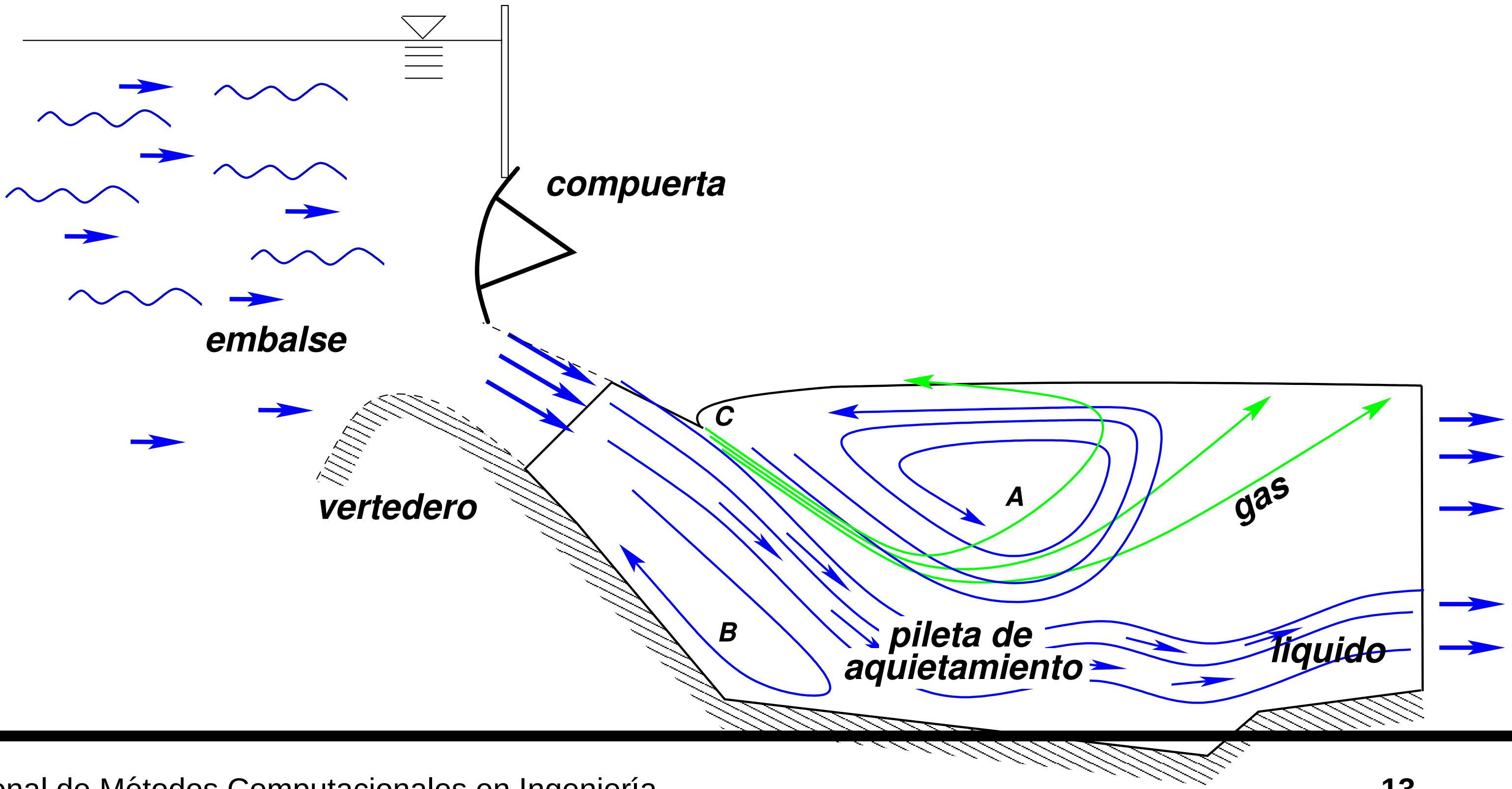
- **Per element physical properties (viscosity, Young modulus,...) can be entered as global, per-elemset or per-element.**
- **Also may be arbitrarily modified at run-time at user level via *"hooks"*. Hooks are a piece of code to be called at well defined points in time. (The concept is borrowed from the Emacs editor). For instance, this allows the user to run some code at the begin/end of a time step, or at the begin/end of the whole run.**
- **Currently hooks must be written in C/C++ (dynamically loaded, with `dlopen()` and friends) or shell script language (and run arbitrarily complex problems from there).**
-

Multi-physics

- **Multi-physics is the ability to manipulate several interacting fields as, for instance, fluid dynamics, elasticity, electromagnetism, transport of scalars, chemical reactions, several phases (multi-phase)...**
- ***Strong interaction* between fields must be implemented monolithically inside an elemset.**
- ***Weak interaction* between fields should be able to be added at the user level, via *hooks*.**

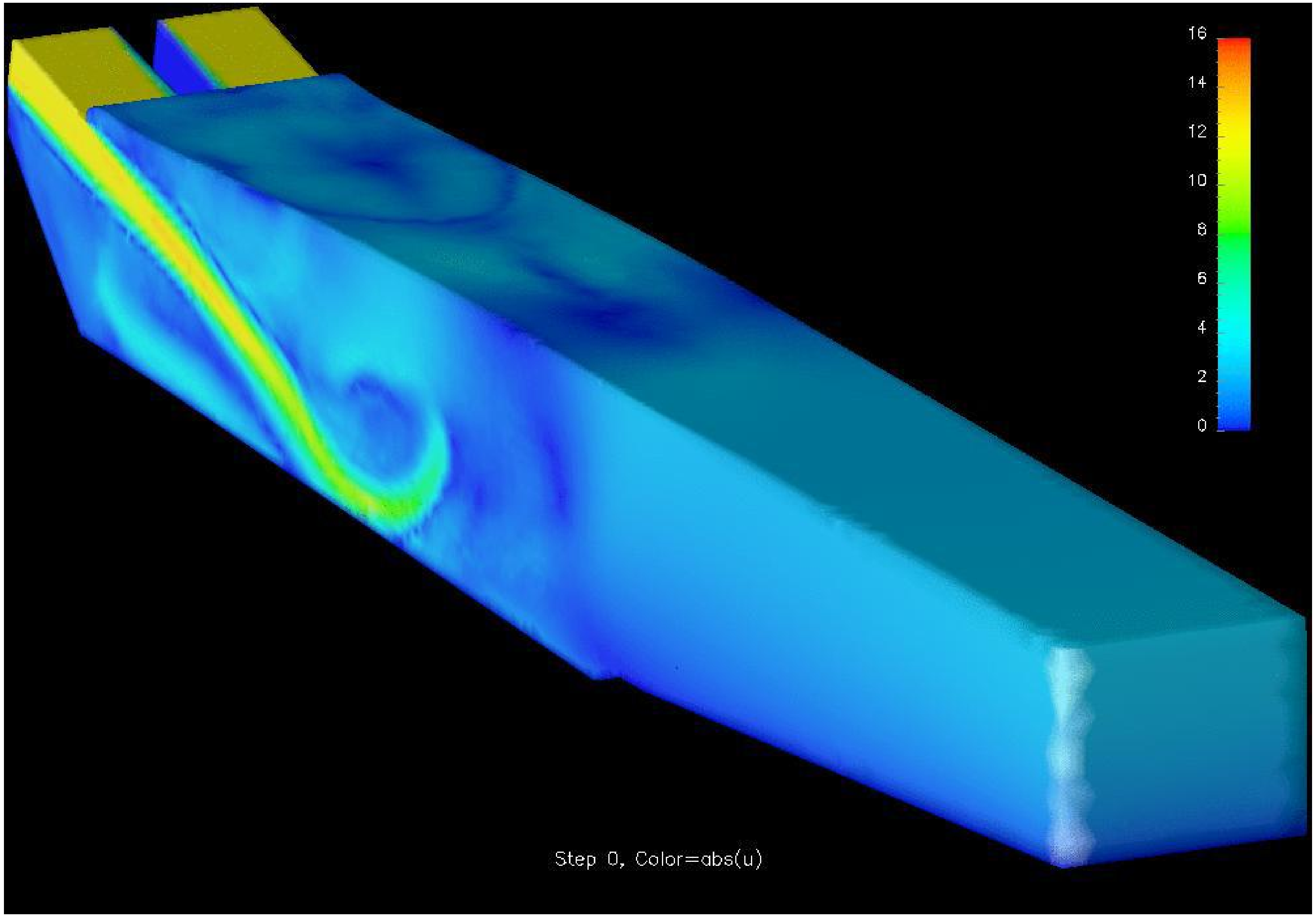
Fluid dynamics with reaction and transport

- **Jet impinging on pool produces high bubble content (foam). High energy jet drags bubbles to the bottom of the pool. Dilution of O2/N2 from gas phase to liquid phase is promoted by high pressures. Bubbles quickly return to air by buoyancy but high concentration of O2/N2 in the liquid remains for long distances downstream.**



Fluid dynamics with reaction and transport (cont.)

- **Model predicts concentration of O2/N2.**
- **The model includes solving the momentum equation and continuity for the (continuous) liquid phase. Driving force for the movement of water in the pool is the impinging jet and bubble buoyancy.**
- **Momentum eq. for gas phase may be treated as a restriction (algebraic model) or as another evolution equation.**
- **Solve transport eq. for bubble number density.**
- **Transport of O2/N2 in the liquid is solved, with reaction terms involving the difference in O2/N2 concentration at the gas phase and liquid phase, bubble density, etc...**
- **Has $2 \cdot n_d + 2$ unknown fields and equations.**
- **May be solved monolithic or staggered in time: advance fluid dynamics, then dilute gas concentration.**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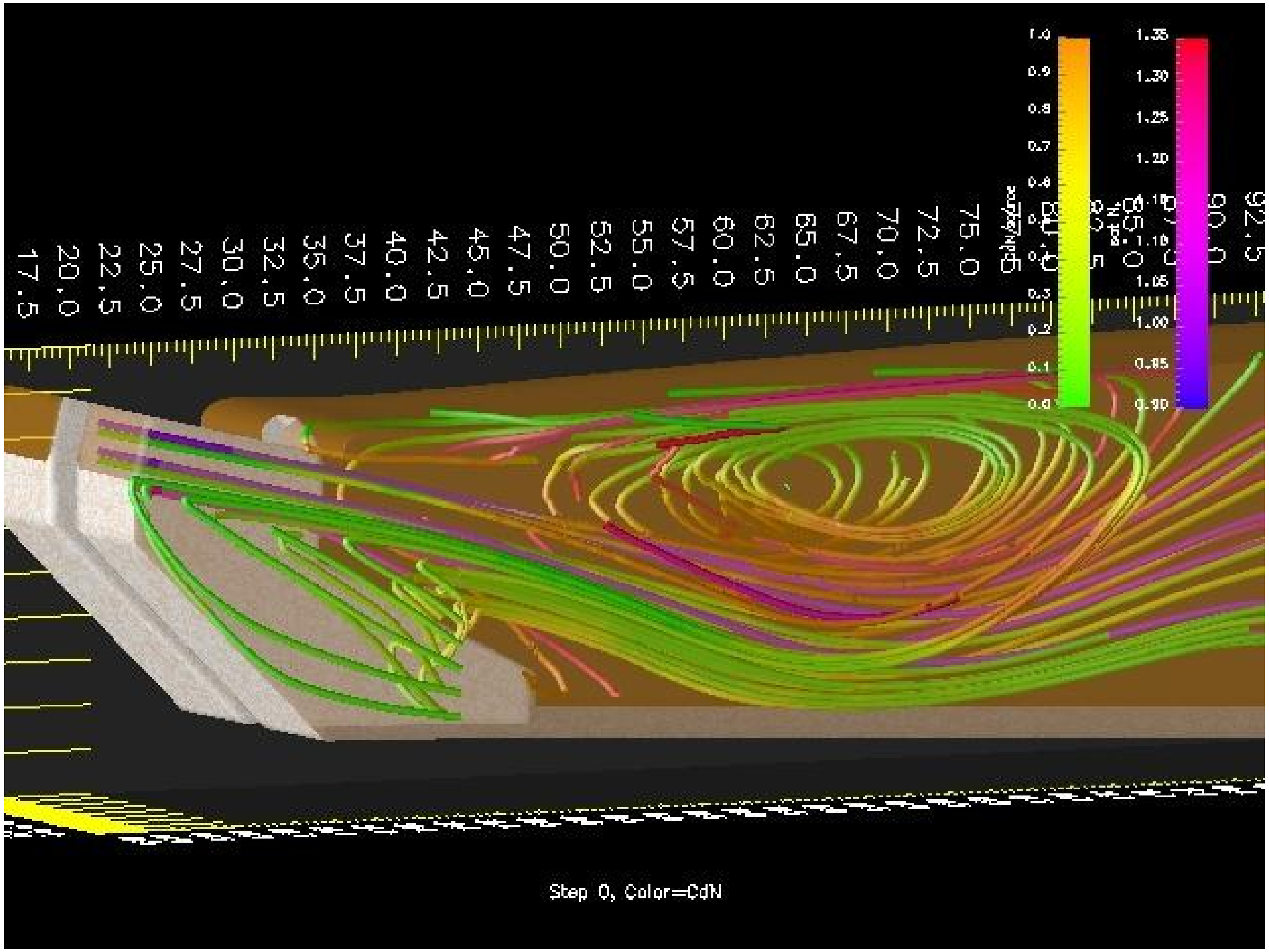
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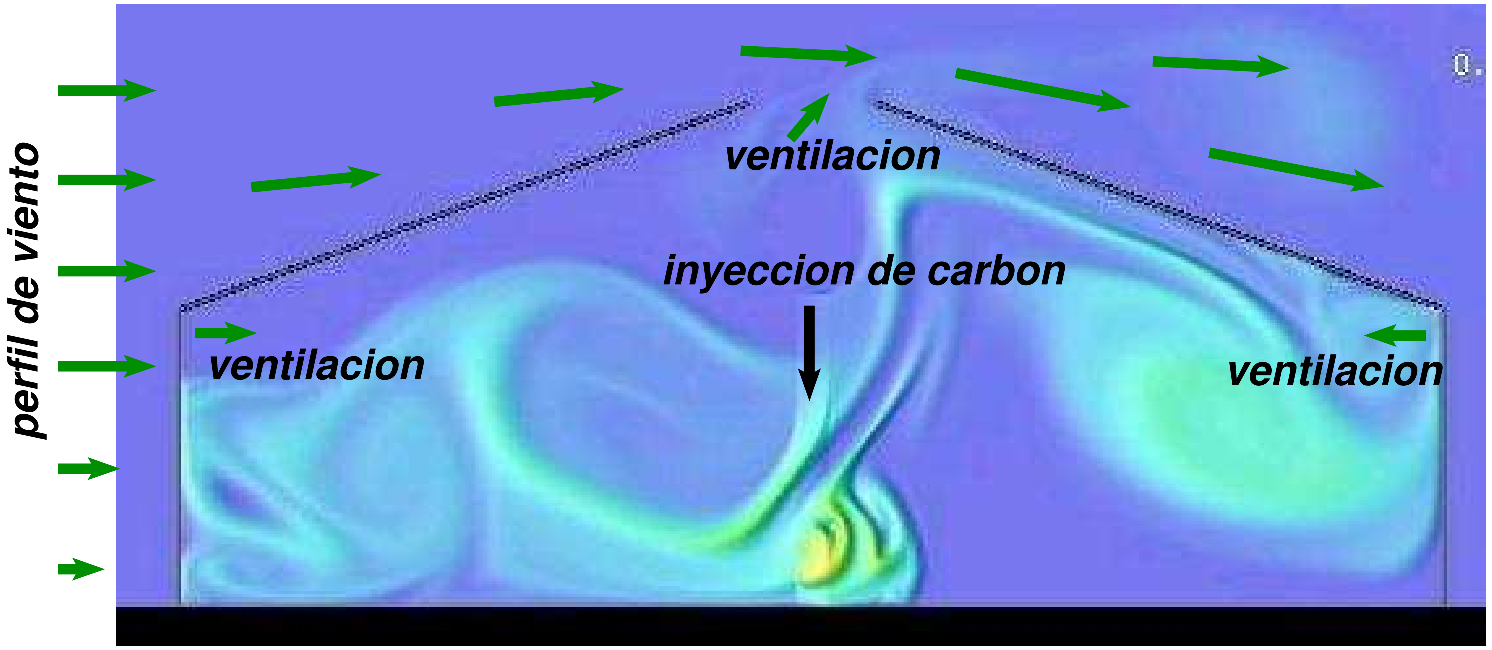
Multi-phase flow gas/solid

Multi-phase gas/solid flow: **Coke processing facility want to assess total amount of particle emission under several conditions (forced and natural convection).**



Multi-phase flow gas/solid (cont.)

- **Solve momentum equations and continuity for air velocity field.**
- **Solve momentum equations for solid particle velocity field or assume algebraic slip model.**
- **Solve particle number transport equation.**
- **May use several particle sizes (one scalar unknown field for each particle size).**

Scripting via extension languages

- **Currently, user data file has a tree-like data structure with nodes meaning of the form (key,value) assignments. Keys and values are strings, and processed internally in order to obtain other entities as integers, doubles, arrays, etc...**
- **Some basic preprocessing is provided internally (includes of large files). Also via an external preprocessor (`ePerl`, similar to `cpp`) for instance for evaluation of expressions, conditional processing, ...**

Scripting via extension languages (cont.)

- **As the syntax of the user data files grew in complexity and more preprocessing is needed (calling functions, system calls...) the syntax *evolves eventually in a language*.**
-

```
global_options

alpha 1. # Integration rule param.

#if !$restart # Conditional processing...
nstep 100000
#else
nstep 1
#endif

tol_newton 1e-10 # Iterative parameters
atol 0
rtol 1e-7
viscosity <:=$U*$L/$Re:> # handle math exps
...
```

Scripting via extension languages (cont.)

Adding features to the user data file syntax and making it a language has many disadvantages.

- **Developer has to define a correct language (syntax, ...) and implement it.**
- **Users have to learn a new language/syntax.**

This happened with a series of Open Source projects (Apache, PHP, Perl, ...). Developers started with a small language definition and ended with a full featured language. A better solution is to use an already existing high level scripting language and extend it with the functions of the new library. In this way the user needs not to deal with coding in a low level language like C/C++ directly. Candidates for extension language are Perl, Python, Lisp/Scheme, Octave...

Scripting via extension languages (cont.)

The subject was at the heart of a war over the net (the *“Tcl war”*, see `http://www.vanderburg.org/Tcl/war/`) and the Free Software Foundation proposed to design a language specific to be an extension language for Free Software projects. This is Guile, a complete implementation of the Scheme language, a dialect of Lisp. Advantages of Guile are

- **It implements Scheme a full featured language. It implements dynamic typing, supports functional programming, has first class procedures, hygienic macros, first class continuations. There are many implementations (interpreters) of Scheme, Guile is just one of them.**
- **It is the extension language proposed by the FSF.**
- **Full support for loading C functions in libraries.**
- **Can call C functions from Scheme and vice-versa.**

Scripting via extension languages (cont.)

User data file will be a Guile/Scheme script

```
(use-modules (petsc-fem base))
(use-modules (petsc-fem ns))
(use-modules (petsc-fem elasticity))

(define global-options
  ‘(alpha . 1.0) ;;; Integration rule param.
  (nstep . ,(if restart 1000 1)) ;;; Cond. proc. . .
  (tol-newton . 1e-10) ;;; Iterative parameters
  (atol . 0)
  (rtol . 1e-7)
  ;;; Handles arbitrarily complex math exps
  (viscosity . ,(/ (* rho U L) Re)))
(define coords (elemset-load "./coords.dat"))
(define elemset (elemset-load "./connect.dat"))
(define ns-problem
  (ns-init coords elemset global-options))
. . .
```

Scripting via extension languages (cont.)

- **Currently best candidates are Scheme and Python.**
- **Written wrappers for MPI and PETSc libraries in Python (Lisandro Dalcín). [“MPI for Python”, Journal of Parallel and Distributed Computing, (article in press, available online 6/4/2005). Can exchange arbitrary Python objects between processors (via `pickle` module).**
- **Basic MPI wrappers in Scheme (only sends/receives special vector objects).**

```
(use-modules (mpi))
(use-modules (dvector))
(mpi-initialize)

;;; Get rank and size
(define my-rank (mpi-rank))
(define size (mpi-size))

;;; Standard parallel hello...
(format t "Hello world I am ~A of ~A\n" my-rank size)

;;; Define vectors v,w, fill v with random
(define N 1000)
(define v (make-dvdbl 1000))
(define w (make-dvdbl 1000))
(dv-rand! v)

;;; Rotates data (sends to myrank+1 and
;;; receives from myrank-1, cyclically)
(cond ((even? my-rank)
       (mpi-send v (modulo (+ my-rank 1) size))
       (mpi-recv w (modulo (- my-rank 1) size)))
      (else
       (mpi-recv w (modulo (- my-rank 1) size)))
       (mpi-send v (modulo (+ my-rank 1) size)))

(mpi-finalize)
```

Functional programming style

```
;;; Saves state file to disk
;;; each 10 time steps
(define nsave 10)

;;; Save each 10 or if large variations in
;;; state vector are detected
(define nsave
 (lambda (step)
  (if (or (= (modulo step 10) )
          (check-state step)))))
```

Functional programming style

Functional programming promotes intermix of code and data (CODE=DATA slogan).

```
;;; Saves state file to disk
;;; each 10 time steps
(define nsave 10)

;;; Save each 10 or if large variations in
;;; state vector are detected
(define nsave
  (lambda (step)
    (if (or (= (modulo step 10) )
             (check-state step)))))
```

Functional programming style (cont.)

```
(define visco 1e-3) ;;; Fixed value for viscosity

(define visco  ;;; Use Sutherland's law
  (sutherland-law 1e-3 300 110 120))

;;; This takes the physical parameters
;;; and returns a function of temperature.
(define (sutherland-law muinf Tinf T1 T2 expo)
  (let ((T1 T1) (T2 T2) (expo expo))
    (lambda (T)
          (if (< T T2)
              (* (muinf (/ T Tinf)))
              (* muinf
                 (/ T2 Tinf)
                 (expt (/ T T2) expo)
                 (/ (+ Tinf T1) (T T1))))))))
```

Absorbing boundary conditions

Well known theory and practice for advective systems say that at a boundary *the number of Dirichlet conditions should be equal to the number of incoming characteristics*.

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathcal{F}_{c,j}(\mathbf{U})}{\partial x_j} = 0$$

$$A_{c,j} = \frac{\partial \mathcal{F}_{c,j}(\mathbf{U})}{\partial \mathbf{U}}, \qquad \text{advective Jacobian}$$

Nbr. of incoming characteristics $= \mathrm{sum}(\mathrm{eig}(\mathbf{A}\cdot\hat{\mathbf{n}}) < 0)$

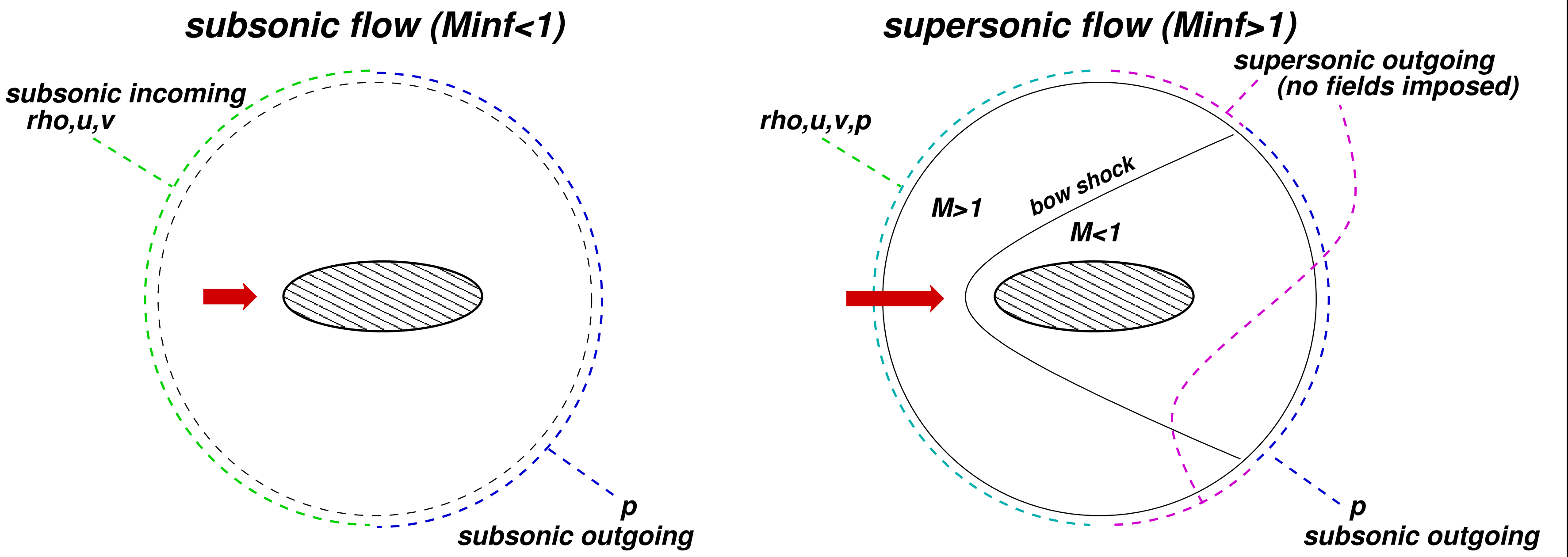
$\hat{\mathbf{n}}$ **is the exterior normal.**

Adding extra Dirichlet conditions leads to spurious shocks, and lack of a Dirichlet conditions leads to instability.

Absorbing boundary conditions (cont.)

For simple scalar advection problems the Jacobian is the transport velocity. The rule is then to check the projection of velocity onto the exterior normal.

For more complex flows (i.e. with *non diagonalizable Jacobians*, as gas dynamics or shallow water eqs.) the number of incoming characteristics may be approx. predicted from the flow conditions.



Absorbing boundary conditions

However, this kind of conditions are, generally, *reflective*. First order absorbing boundary conditions may be constructed by imposing exactly the components along the incoming characteristics.

$$\mathbf{\Pi}^{-}(\mathbf{U}_{\mathrm{ref}})\,(\mathbf{U}-\mathbf{U}_{\mathrm{ref}})=0.$$

$\mathbf{\Pi}^{-}$ **is the projection operator onto incoming characteristics. It can be obtained straightforwardly from the projected Jacobian.**

This assumes linearization of the equations around a state $\mathrm{U}_{\mathrm{ref}}$. For linear problems $\mathbf{A}_{c,j}$ do not depend on U, and then neither the projection operator, so that absorbing boundary conditions coefficients are constant.

Absorbing boundary conditions (cont.)

For non-linear problems the Jacobian and projection operator may vary and then the above mentioned b.c.'s are not fully absorbing.

In some cases the concept of characteristic component may be extended to the non-linear case: the *"Riemann invariants"*. Fully absorbing boundary conditions could be written in terms of the invariants:

$$w_j = w_{\mathrm{ref},j}, \quad \textbf{if } w_j \textbf{ is an incoming R.I.}$$

- **R.I. are computed analytically. There are no automatic (numerical) techniques to compute them. (They amount to compute an integral in phase space *along a specific path*).**
- **R.I. are known for shallow water, channel flow (for rectangular and triangular channel shape). For gas dynamics the well known R.I. in fact are invariants only under isentropic conditions (i.e. not truly invariant).**

Absorbing boundary conditions (cont.)

Search for an absorbing boundary condition that

- **Fully absorbent (i.e. in non-linear conditions).**
- **Can be computed numerically (no need of analytic expressions like R.I.)**

Solution: **Use previous state as reference state ($\mathrm{U}_{\rm ref} = \mathrm{U}^n$, $n =$ time step number).**

$$\mathbf{\Pi}^-(\mathbf{U}^n)\,(\mathbf{U}^{n+1} - \mathbf{U}^n) = 0.$$

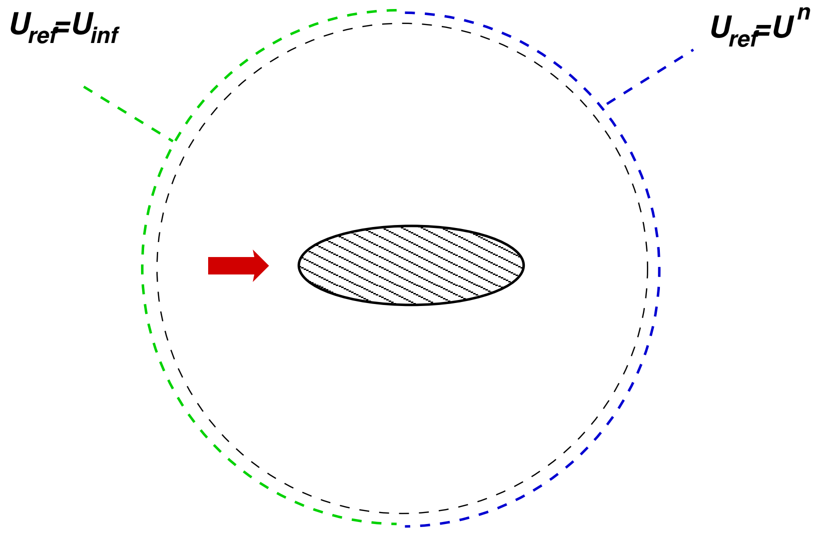
As $\mathrm{U}^{n+1} - \mathrm{U}^n$ is usually small, linearization is valid.

Absorbing boundary conditions (cont.)

Disadvantage: **Flow conditions are only determined from the initial state!! No external information comes from the outside.**

Solution: use a combination of linear/R.I. b.c.'s on incoming boundaries and use fully non-linear a.b.c's with previous state as reference state at the outlet.

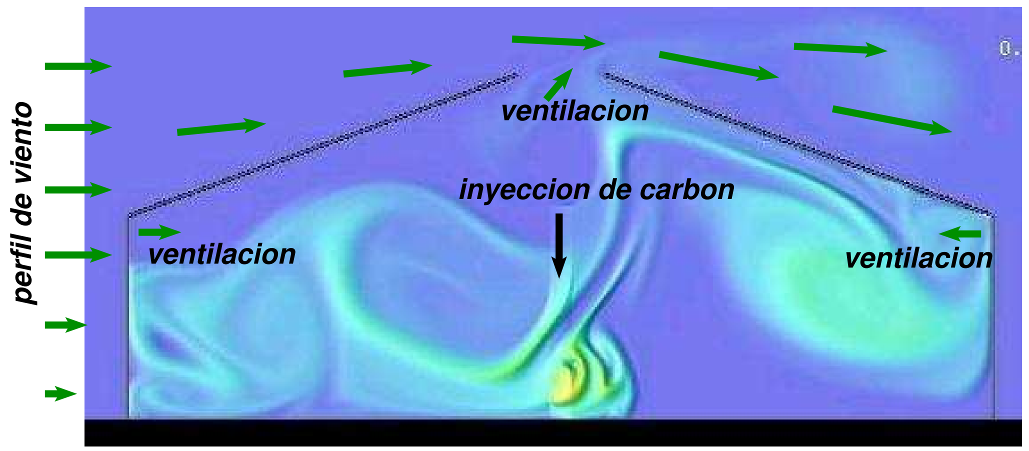
subsonisupersonic flow



Dynamic boundary conditions

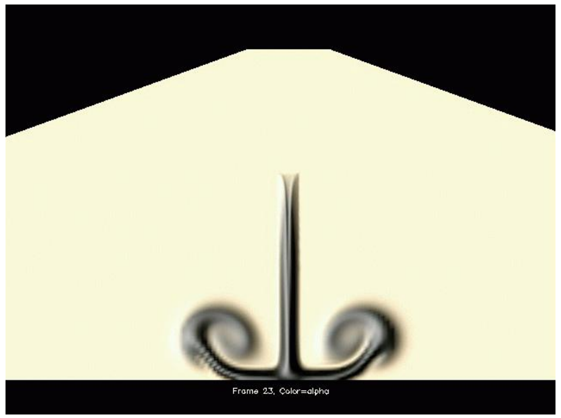
Finally, there is a last twist in the use of absorbing boundary conditions. As the flow is computed it may happen that the number of characteristics changes in time. Two examples follow.

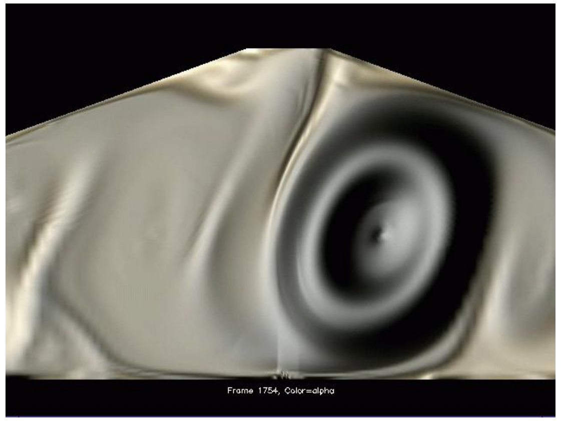
Think at transport of a scalar on top of a velocity field obtained by an incompressible Navier-Stokes solver (not truly that in the example since both systems are coupled). If the exterior flow is not modeled then flow at the top opening may be reverted.

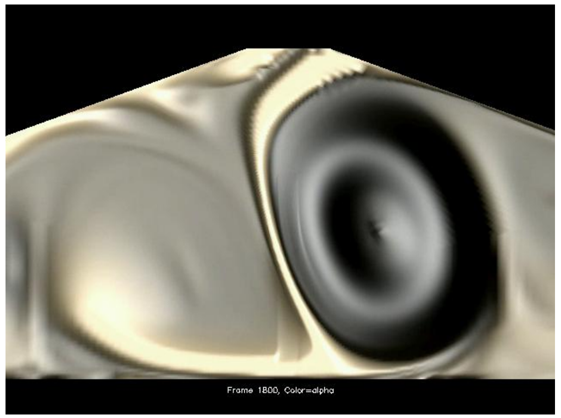


Dynamic boundary conditions (cont.)

If the interior is modeled only, then it's natural to leave concentration free at the top opening. However the flow can revert at some portions of the opening producing a large incoming of undetermined values (in practice large negative concentrations are observed). Imposing a value at the opening is stable but would lead to a spurious discontinuity at the outlet.





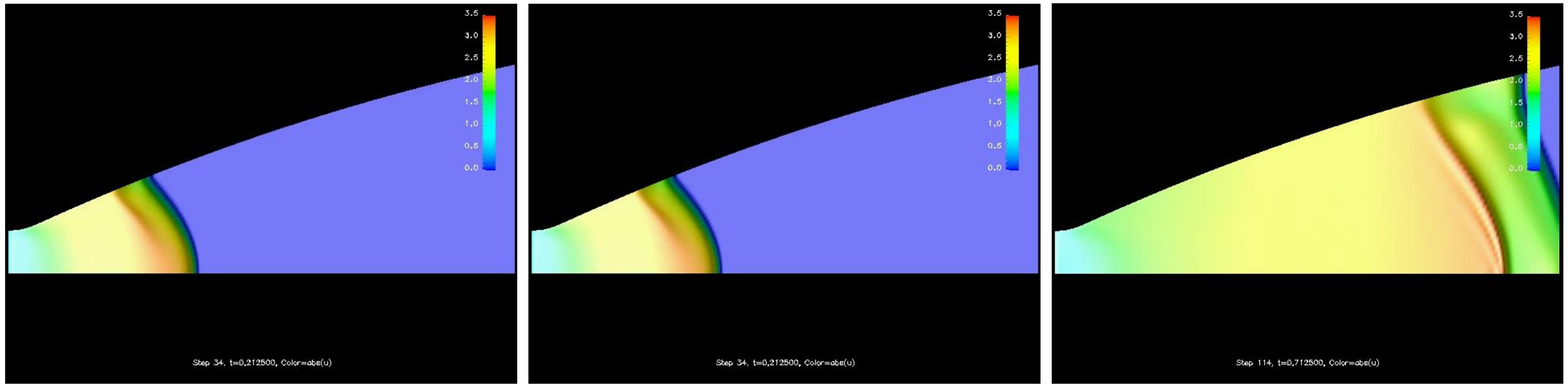


The ideal would be to switch *dynamically* from one condition to the other during the computation.

Dynamic boundary conditions (cont.)

Nozzle chamber fill

The case is the ignition of a rocket launcher nozzle in a low pressure atmosphere. The fluid is initially at rest (143 Pa, 262 $^\circ\mathrm{K}$). At time $t = 0$ a membrane at the throat is broken. Behind the membrane there is a reservoir at 6×10^5 Pa, $4170^\circ\mathrm{K}$. A strong shock (intensity p_1/p_2¿1000) propagates from the throat to the outlet. The gas is assumed as ideal ($\gamma = 1.17$). In the steady state a supersonic flow with a max. Mach of 4 at the outlet is found. The objective of the simulation is to determine the time needed to fill the chamber ($< 1\mathrm{msec}$) and the final steady flow.



Dynamic boundary conditions (cont.)

We impose density, pressure and tangential velocity at inlet (assuming subsonic inlet), slip condition at the nozzle wall. The problem is with the outlet boundary. Initially the flow is subsonic (fluid at rest) there, and switches to supersonic. The rule dictaminates to impose 1 condition, as a subsonic outlet (may be pressure, which is known) and no conditions after (supersonic outlet). If pressure is imposed during the wall computation, then a spurious shock is formed at the outlet.

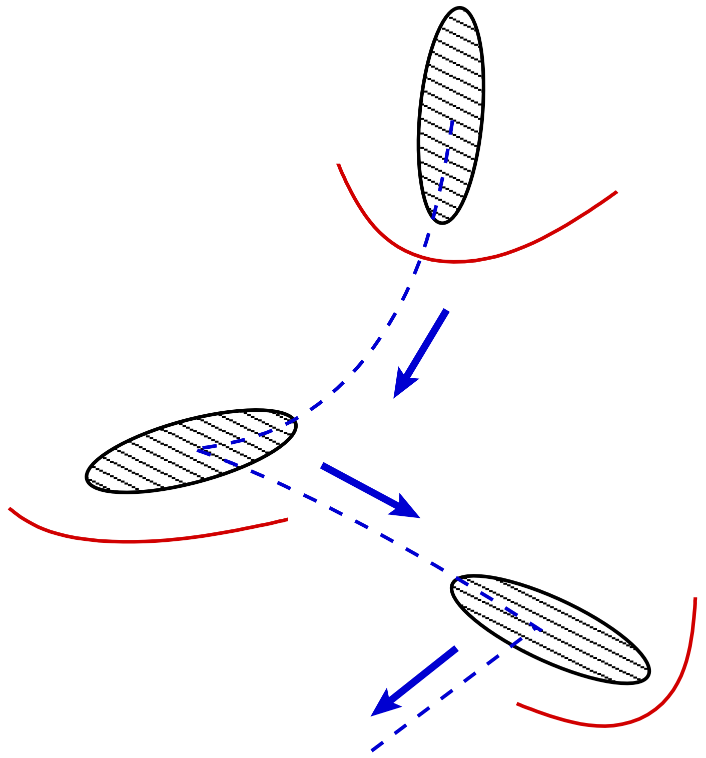
This test case has been contrasted with experimental data obtained at ESTEC/ESA (European Space Research and Technology Centre-European Space Agency, Noordwijk, Holanda). The predicted mean velocity was $2621\ \mathrm{m/s}$ to be compared with the experimental value of $2650 \pm 50\ \mathrm{m/sec}$.

Again, the ideal would be to switch *dynamically* from one condition to the other *during the computation*.

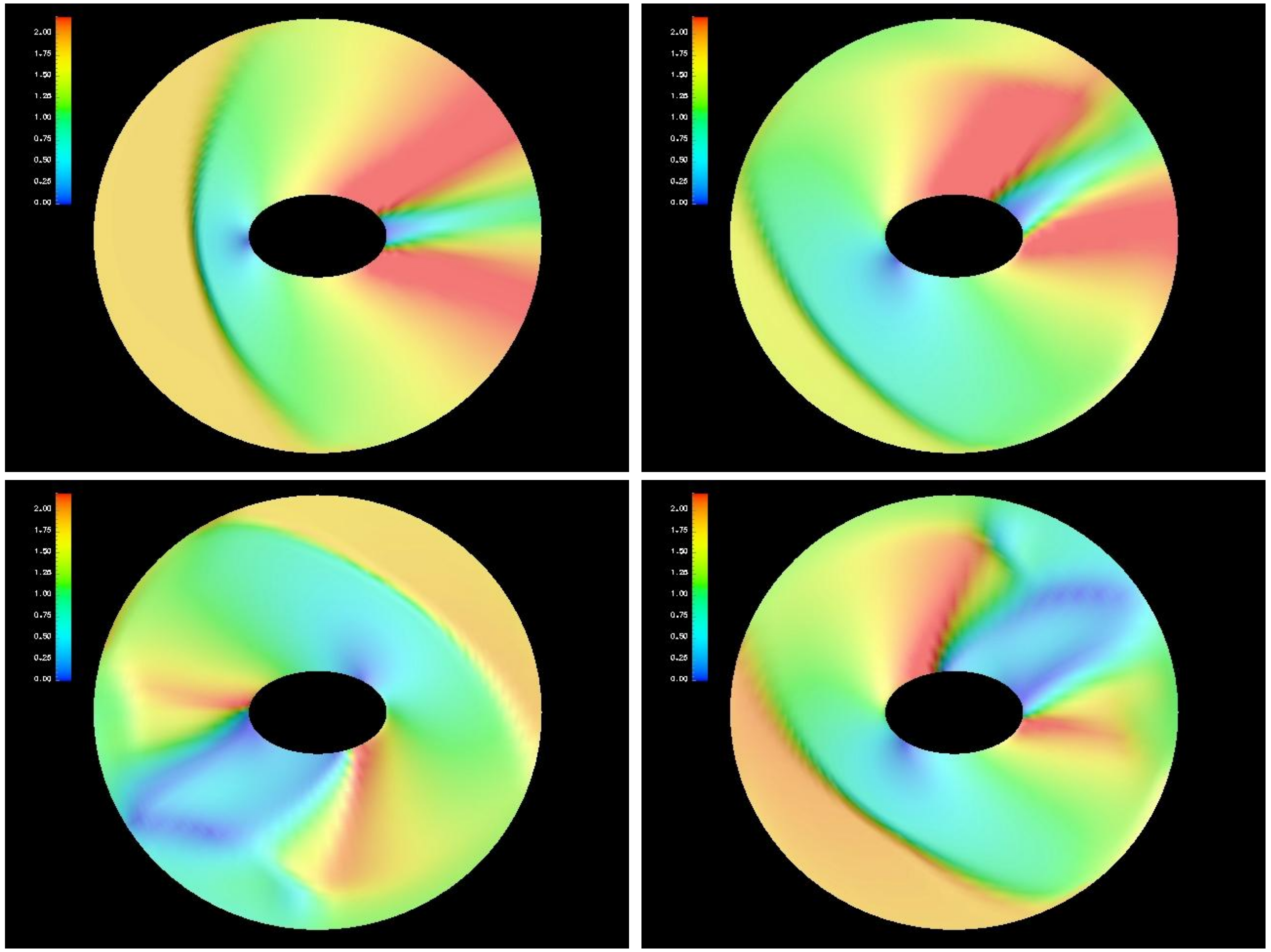
Object falling at supersonic regime

We have an object in free fall, under certain conditions in size and density relation to the surrounding atmosphere it reaches supersonic speeds. At supersonic speeds the principal source of drag is the shock wave, we use slip boundary condition at the body in order to simplify the problem.

We also do the computation in a non-inertial system following the body, so that non-inertial terms (Coriolis, centrifugal, etc...) are added. In this frame some portions of the boundary are alternatively in all the conditions (subsonic incoming, subsonic outgoing, supersonic incoming, supersonic outgoing).
Again, the ideal would be to switch* dynamically *from one condition to the other during the computation.



Object falling at supersonic regime (cont.)



Dynamic boundary conditions

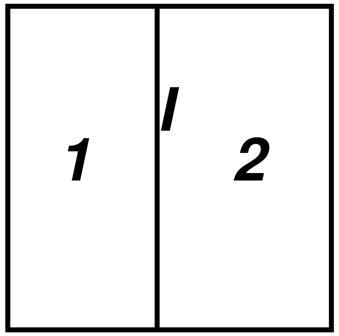
In order to avoid modification of the matrix structure we add dynamic boundary conditions either via Lagrange multipliers or penalization. However this techniques add extra bad conditioning to the system of equations so that special iterative methods are needed.

Parallel solution of large linear systems

- **Direct solvers are highly coupled and don't parallelize well (high communication times). Also they require too much memory, and they asymptotically demand more CPU time than iterative methods even in sequential mode. But they have the advantage that the computational cost do not depend on condition number.**
- **Iteration on the global system of eqs. is highly uncoupled (low communication times) but has low convergence rates, specially for bad conditioned systems.**
- ***"Substructuring"* or *"Domain Decomposition"* methods are somewhat a mixture of both: the problem is solved on each subdomain with a direct method and we iterate on the interface values in order to enforce the equilibrium equations there.**

Global iteration methods

$$\begin{bmatrix} A_{11} & 0 & A_{1I} \\ 0 & A_{22} & A_{2I} \\ A_{I1} & A_{I2} & A_{II} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_I \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_I \end{bmatrix}$$



- **Computing matrix vector operations involve to compute diagonal terms $A_{11}x_1$ and $A_{22}x_2$ in each processor and,**
- **Communicate part of the non-diagonal contributions.**

Global iteration methods (cont.)

Eliminate x_1 and x_2 to arrive to the condensed eq.

$$
\begin{aligned}
(A_{II} - A_{I1} A_{11}^{-1} A_{1I} - A_{I2} A_{22}^{-1} A_{2I})\, x_I \\
&= (b_I - A_{I1} A_{11}^{-1}\, b_1 - A_{I2} A_{22}^{-1}\, b_2) \\
\tilde{A}\, x_I = \tilde{b}
\end{aligned}
$$

Evaluation of $y_I = \tilde{A}\, x_I$ implies

- **Solving the local equilibrium equations in each processor for x_j:** $A_{jj}\, x_j = -A_{jI}\, x_I$
- **Sumation of the interface and local contributions:** $y_I = A_{II}\, x_I + A_{I1}\, x_1 + A_{I2}\, x_2$
- **This method will be referred later as DDM/SCMI (*"Domain Decomposition Method/Schur complement matrix iteration"*).**

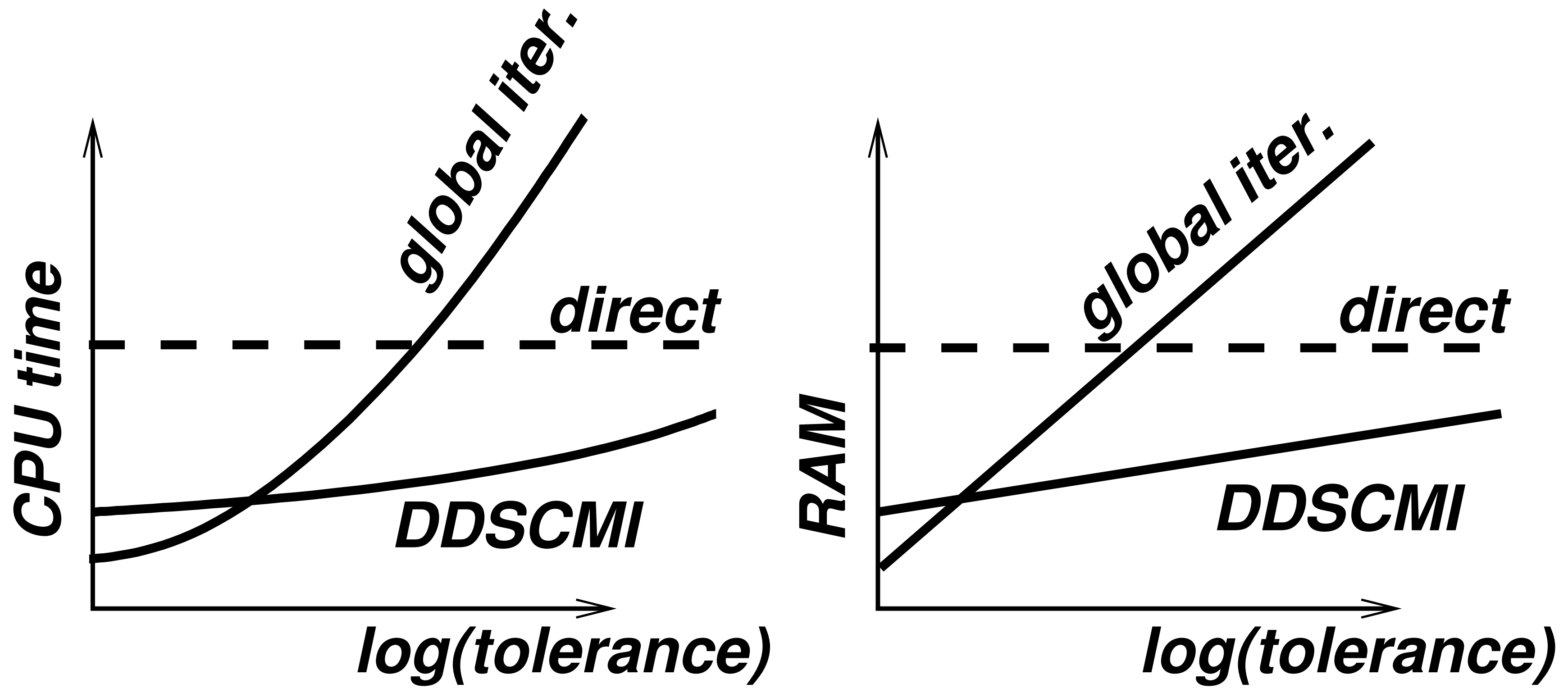
DDM/SCMI vs. Global iter.

- **Iteration on the Schur complement matrix (condensed system) is equivalent to iterate on the subspace where the local nodes (internal to each subdomain) are in equilibrium.**
- **The rate of convergence (per iteration) is improved ☺ due to: a) the condition number of the Schur complement matrix is lower, b) the dimension of the iteration space is lower (non-stationary methods like CG/GMRES tend to accelerate as iteration proceeds). However this is somewhat compensated by factorization time and backsubst. time ☹.**
- **As the iteration count is lower and the iteration space is significantly smaller, RAM requirement for the Krylov space is significantly lower ☺, but this is somewhat compensated by the RAM needed by the factorized internal matrices $LU(A_{jj})$ ☹.**

DDM/SCMI vs. Global iter. (cont.)

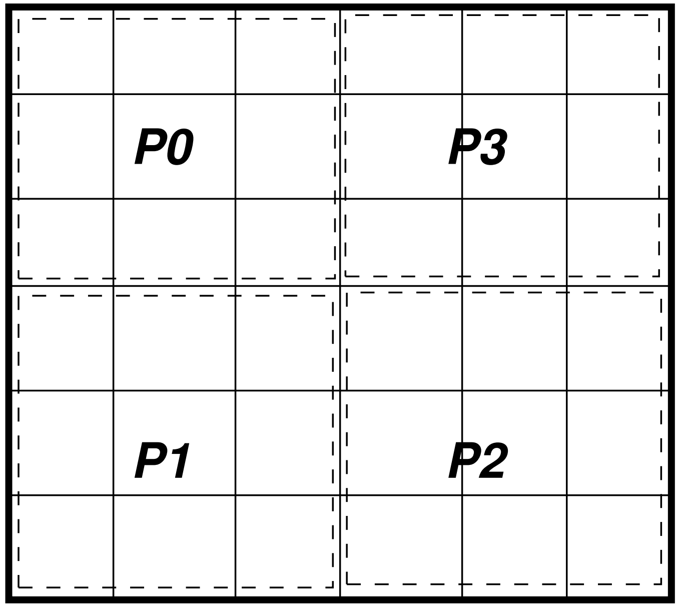
- **Better conditioning of the Schur comp. matrix prevents CG/GMRES convergence break-down ☺**
- **As GMRES CPU time is quadratic in iteration count (orthogonalization stage) and global iteration requires usually more iterations, Schur comp. matrix iteration is comparatively better for lower tolerances (☺/☹).**
- **Global iteration is usually easier to load balance since it is easier to predict computation time accordingly to the number of d.o.f.'s in the subdomain ☹**

DDM/SCMI vs. Global iter. (cont.)



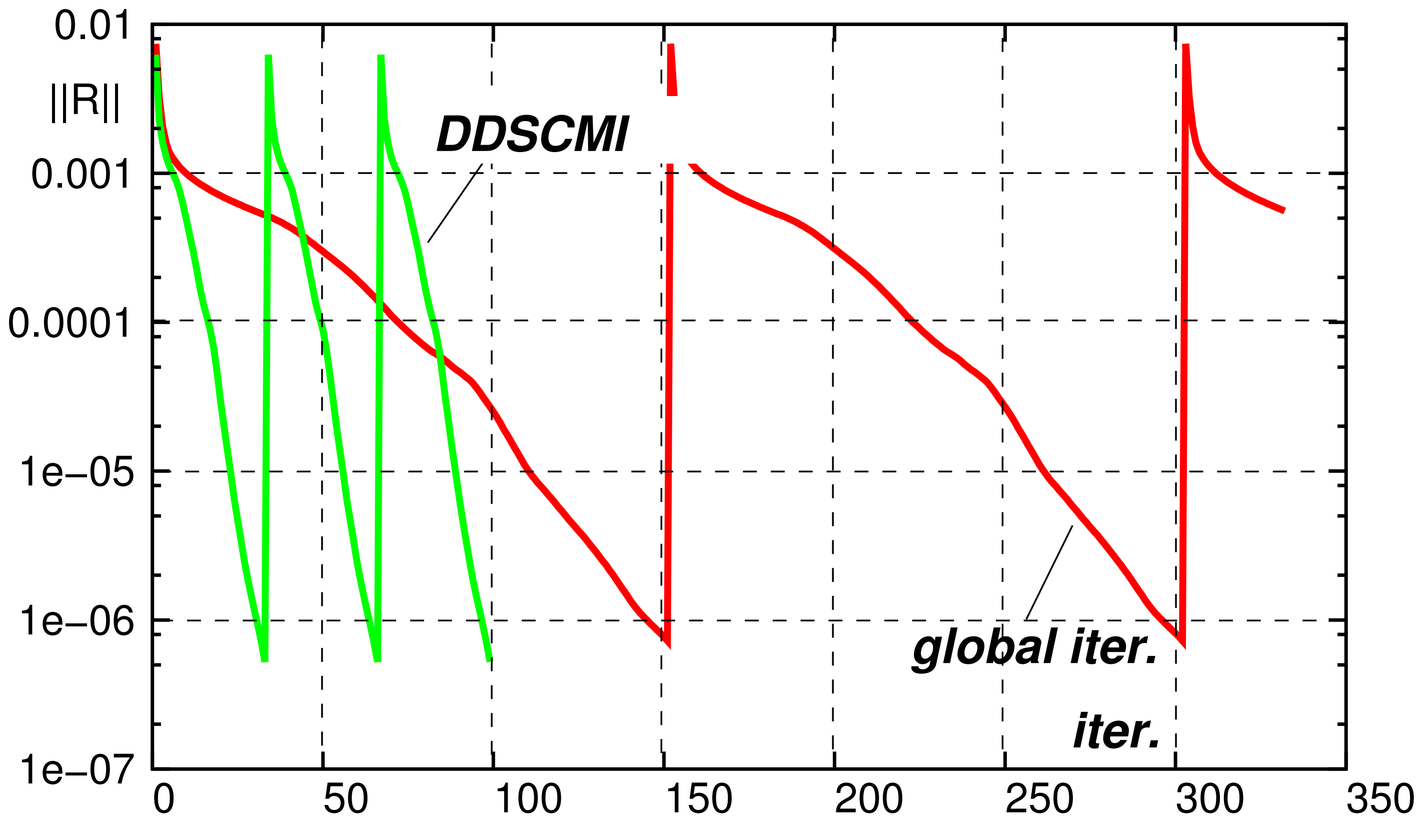
Subpartitioning

- **For large problems, the factorized part of the A_{jj} matrix may exceed the RAM in the processor. So we can further subpartition the domain in the processor in smaller sub-subdomains.**
- **In fact, best efficiency is achieved with relatively small subdomains of 2,000-4,000 d.o.f.'s per subdomain.**



Example. Navier Stokes cubic cavity Re=1000

625,000 tetras mesh, rtol=10^{-4}, NS monolithic, [Tezduyar et.al. TET (SUPG+PSPG) algorithm, CMAME, vol. 95, pp. 221-242, (1992)]



Example. Navier Stokes cubic cavity Re=1000 (cont.)

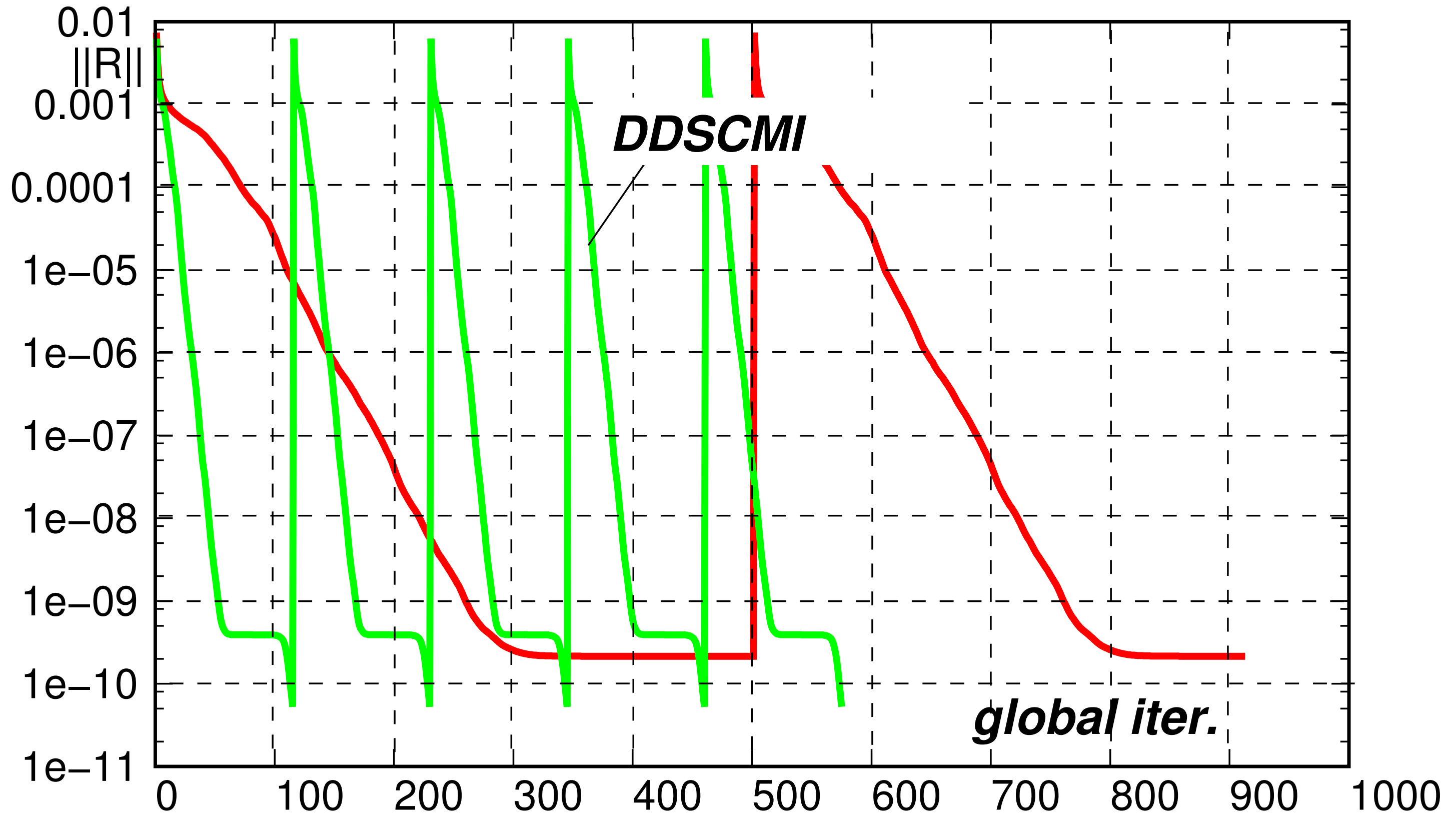
- **Of course, each iteration of DDM/SCMI takes more time, but finally, in average we have**

$$\begin{aligned}\textbf{CPU TIME(DDM/SCMI)} &= \textbf{17.7 secs},\\ \textbf{CPU TIME(Global iteration)} &= \textbf{63.8 secs}\end{aligned}$$

- **Residuals are on the interface for Schur compl, global for Global iter. But vector iteration for the SCM is equivalent to a global vector with null residual on the internal nodes. (So that they are equivalent).**
- **SCMI requires much less communication** ☺

Example. Navier Stokes cubic cavity Re=1000 (cont.)

For a lower tolerance (rtol=10^{-8}), Global iteration breaks down, while DDM/SCMI continues to converge.



Example. Navier Stokes cubic cavity Re=1000 (cont.)

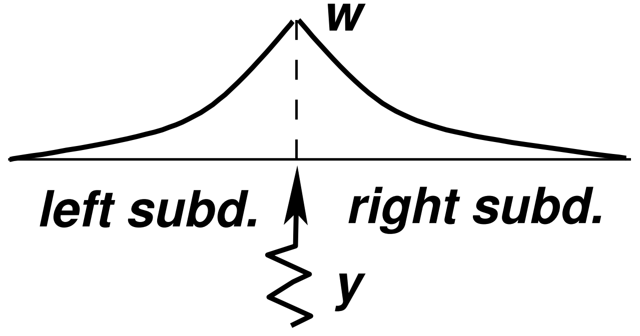
- **Following results obtained with Beowulf cluster Geronimo at CIMEC (see http://www.cimec.org.ar/geronimo). 8 x P4 1.7 Ghz (512MB RIMM (Rambus)).**
- **With DDM/SCMI we can run 2.2 Mtetras with NS monolithic (cubic cavity test) 252secs/iter (linear solution only, to rtol=10^{-4}).**
- **Global iteration crashes (out of memory!) at iteration 122 having converged a factor 5×10^{-3}.**
- **DDM/SCMI is specially suited to stabilized methods, since they are in general worse conditioned. Also when Lagrange multipliers, penalization, strong Darcy terms are used.**

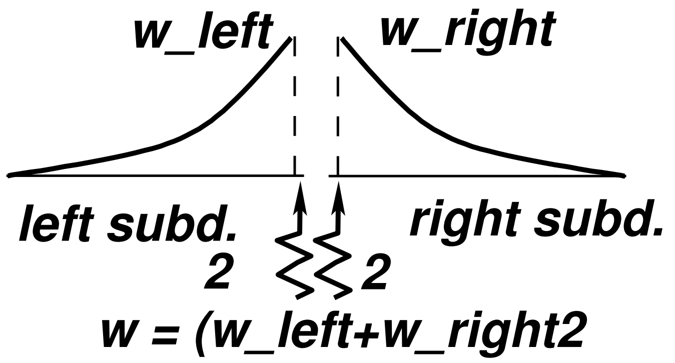
Fractional step solver

- **Predictor and projection steps have $\kappa = O(1)$ are better solved by global iteration (even Richardson).**
- **Poisson step can be solved with DDM/SCMI.** *[Some of the following observations apply in general for symmetric, positive definite operators.]*
- **Better conditioning (than monolithic) makes global iteration more appropriate ☹. As Conjugate Gradient can be used in place of GMRES, CPU time vs. iteration is no more quadratic ☹**
- **Factorized internal subdomain matrices can be stored and no refactorized, so we can use larger internal subdomains (but requires more RAM) ☺**
- **We can solve 4.2 Mtetra mesh in 58sec (Poisson solution time only...) (rtol=10^{-4}, 130 iters.)**

Schur CM preconditioning - NN

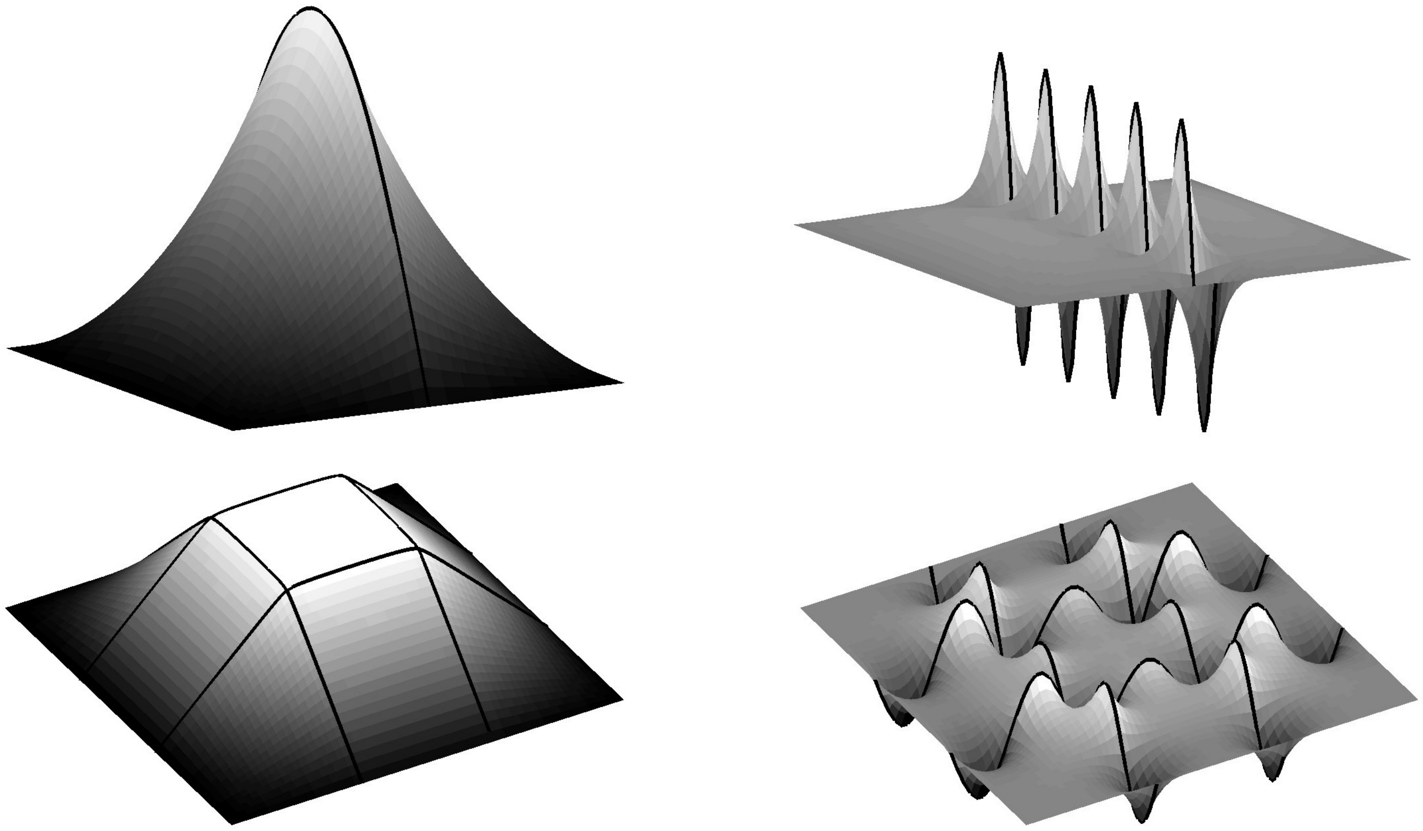
- **In order to further improve SCMI several preconditionings have been developed over years. When solving $\tilde{A}x = \tilde{b}$ a preconditioner should solve $\tilde{A}w = y$ for w in terms of y approximately.**
- **For the Laplace eq. this problem is equivalent to apply a *"concentrated heat flux"* (like a Dirac's δ) y at the interface and solving for the corresponding temperature field. Its trace on the interface is w.**
- **Neumann-Neumann preconditioning amounts to split the heat flux one-half to each side of the interface (${}^1\!/_2 y$ for each subdomain).**





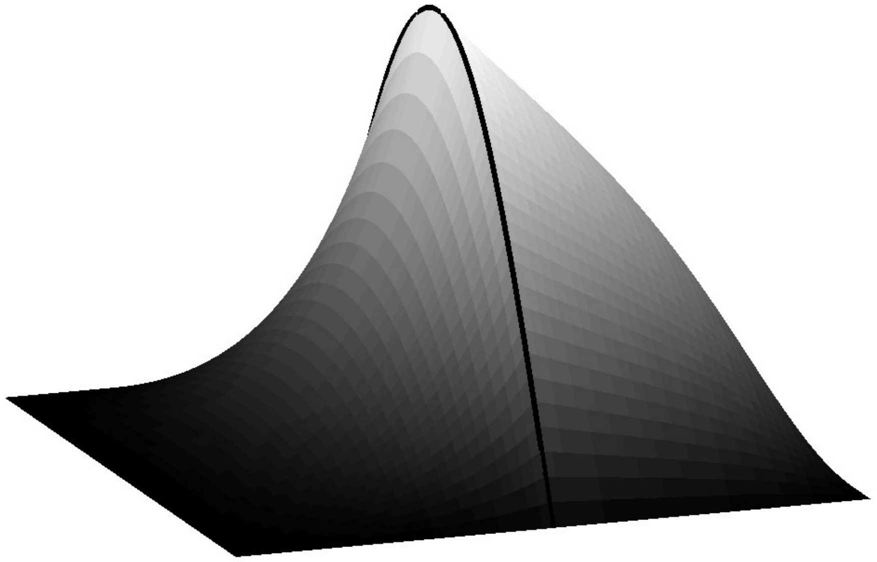
Flux splitting

Neumann-Neumann prec. works well whenever *“equal splitting”* is right: right subdomain equal to left subdomain, symmetric operator... Eigenfunctions of the Stekhlov operator (Schur comp. matrix) are symmetric.



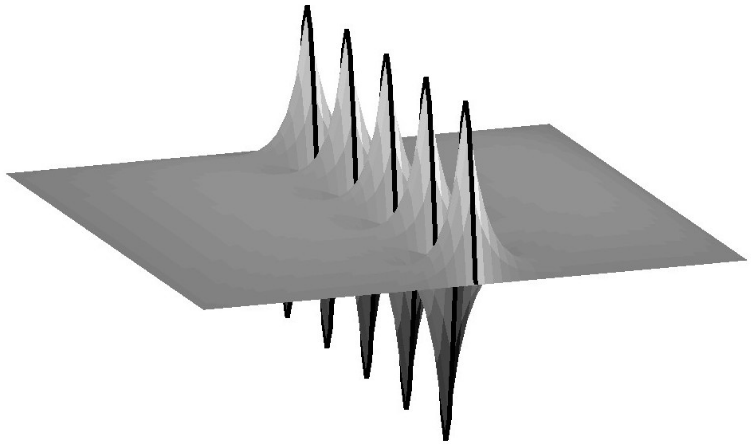
Flux splitting (advective case)

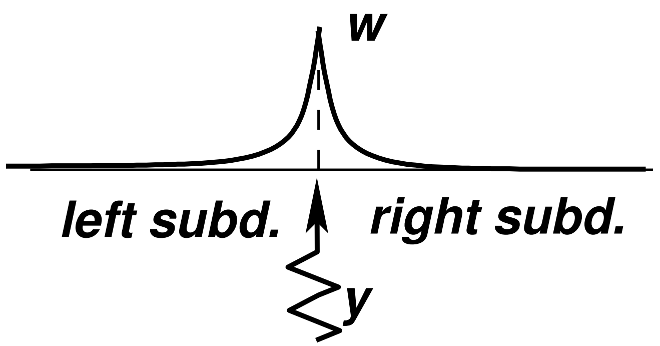
In the presence of advection splitting is biased towards the down-wind sub-domain. Eigenfunctions are no more symmetric.

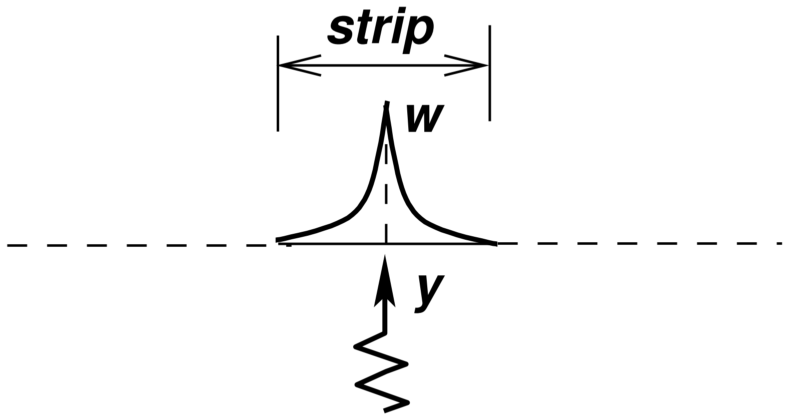


Interface strip preconditioner

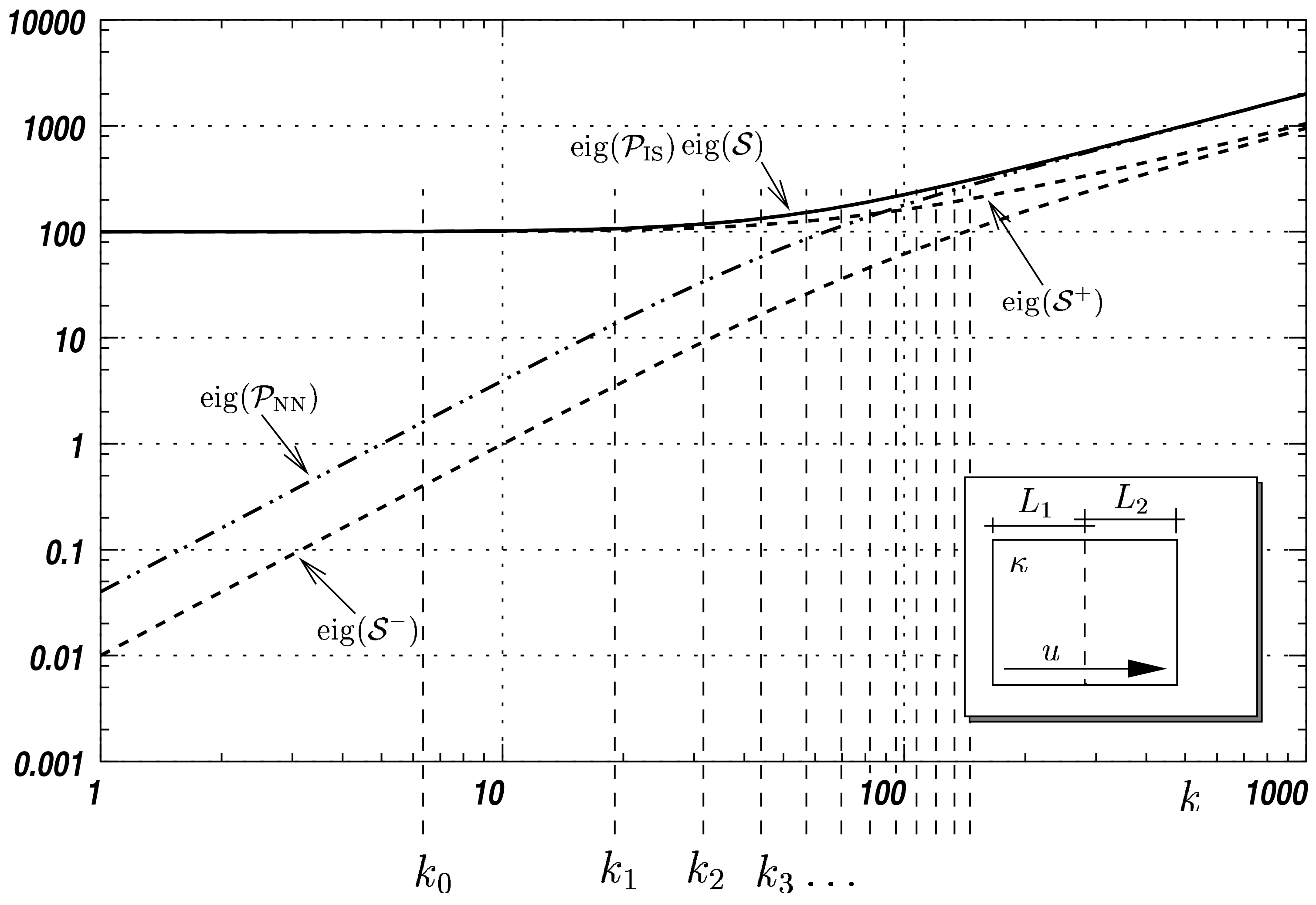
- **For high-frequency modes (high eigenvalues) the eigenfunctions concentrate near the interface.**
- **ISP: Solve the problem in a narrow strip around the interface**







Strongly advective case (Pe=50



Condition number, 50x50 mesh

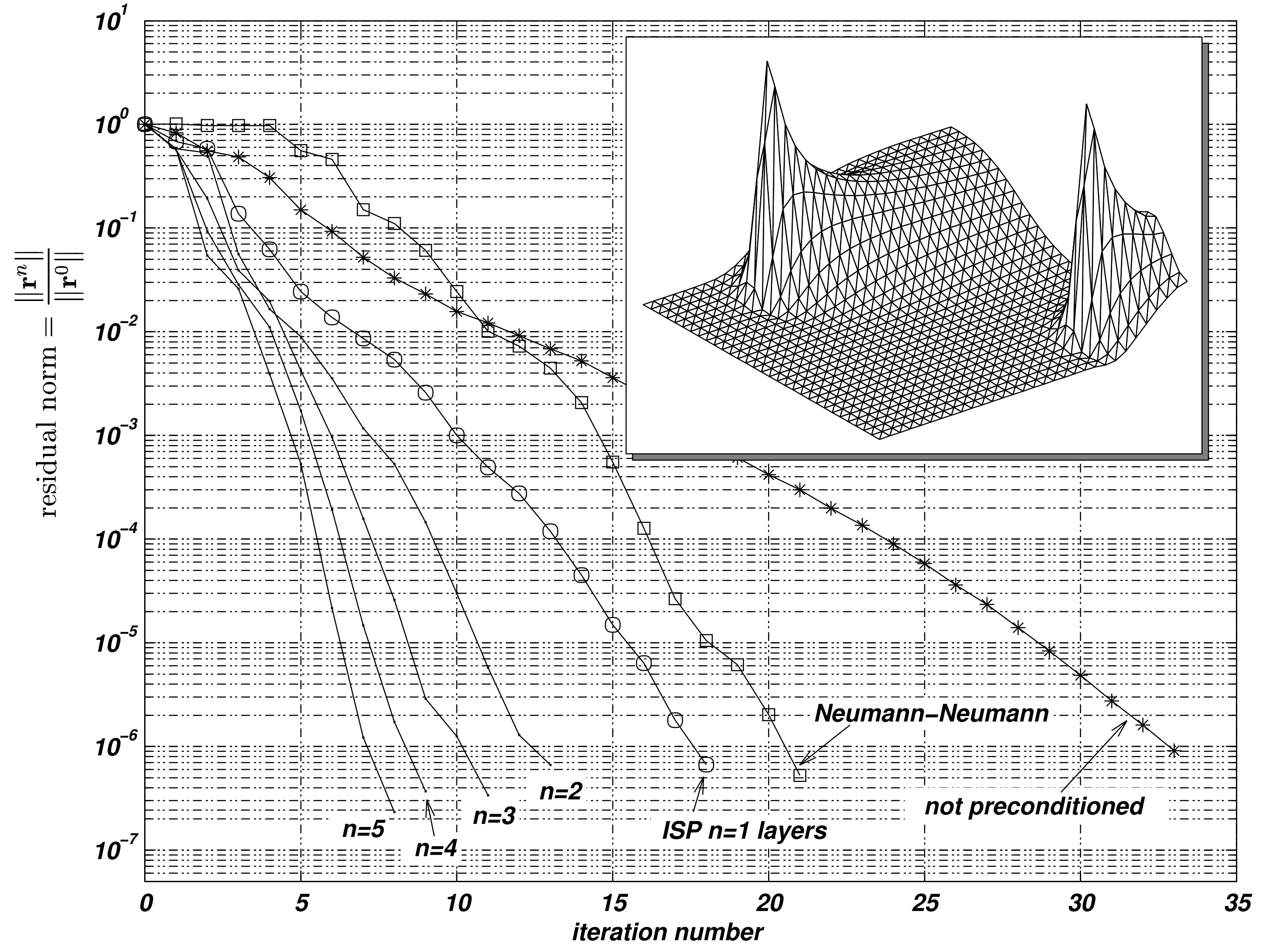
u	$\mathrm{cond}(\mathcal{S})$	$\mathrm{cond}(\mathcal{P}_{\mathrm{NN}}^{-1}\mathcal{S})$	$\mathrm{cond}(\mathcal{P}_{\mathrm{IS}}^{-1}\mathcal{S})$
0	**41.00**	**1.00**	**4.92**
1	**40.86**	**1.02**	**4.88**
10	**23.81**	**3.44**	**2.92**
50	**5.62**	**64.20**	**1.08**

Cuadro 1: Condition number for the Stekhlov operator and several preconditio-ners for a mesh of 50×50 elements.

Condition number, 100x100 mesh

u	$\mathrm{cond}(\mathcal{S})$	$\mathrm{cond}(\mathcal{P}_{\mathrm{NN}}^{-1}\mathcal{S})$	$\mathrm{cond}(\mathcal{P}_{\mathrm{IS}}^{-1}\mathcal{S})$
0	**88.50**	**1.00**	**4.92**
1	**81.80**	**1.02**	**4.88**
10	**47.63**	**3.44**	**2.92**
50	**11.23**	**64.20**	**1.08**

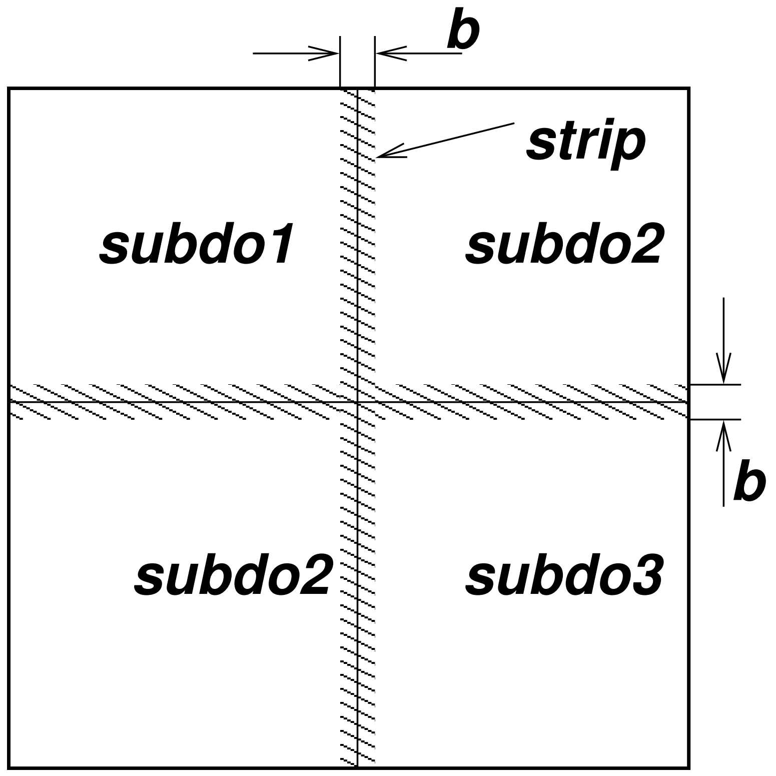
Cuadro 2: Condition number for the Stekhlov operator and several preconditioners for a mesh of 100×100 elements.



$\text{residual norm} = \frac{\|\mathbf{r}^n\|}{\|\mathbf{r}^0\|}$
iteration number
Neumann−Neumann
not preconditioned
ISP n=1 layers
n=2
n=3
n=4
n=5

ISP features

- **Better than NN for strong advective case ☺(NN can improve splitting, but here splitting should depend on wave-length)**
- **No floating subdomains.**
- **Cost depends on strip width. Good conditioning can be obtained with thin strips ($\ll$NN) ☺**
- **Solution of strip problem should be done iteratively. Two possibilities: communicates (weakly coupled) or doesn't communicate (diagonal dominant).**



ISP Implementation

- ISP matrix is ***"global"*** (has elements in all processors): can't be inverted with a direct solver.
- Iterative solution can't use a CG/GMRES solver (can't nest CG/GMRES inside CG/GMRES)
- Use either preconditioned Richardson iteration or disconnect (i.e. modify) ISP matrix in some way in order to get a more disconnected matrix and use a direct method.
- Only preconditioned Richardson iteration is currently implemented in PETSc-FEM.

Cubic cavity

- **Use N^3 regular hexahedral mesh or $5N^3$ tetra mesh.**
- **Very dense connectivity (high LU band-width, strong 3D).**
- **Covers many real flow features (separation, boundary layers...)**
- **For N=30 (135Ktet), using 128 subdomains, 50 % savings in CPU time, 25 % savings in RAM.**

N=30 cubic cavity stat.

nlay	iters
0	340
1	148
2	38

Conclusions

- **Domain Decomposition + iteration on the Schur complement matrix is an efficient algorithm for solving large linear systems in parallel or sequentially.**
- **Specially suited for ill-conditioned problems (stabilized methods, Lagrange multipliers, penalization, strong Darcy terms...)**
- **Interface strip preconditioner improves convergence, specially for advection dominated problems or floating subdomains.**

Acknowledgment

This work has received financial support from Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET, Argentina, grants PIP 0198/98), Universidad Nacional del Litoral (Argentina, grants CAI+D 2000/43) and ANPCyT (Argentina, grants PICT 6973/99, PID-74/99, PICT Lambda/2003, PME 209/2003). We made extensive use of freely distributed software as GNU/Linux OS, MPI, PETSc, gcc compilers, Guile, Python, Octave, Open-DX among many others.