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High-performance large eddy simulation of incompressible turbulent flows

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Joint work with

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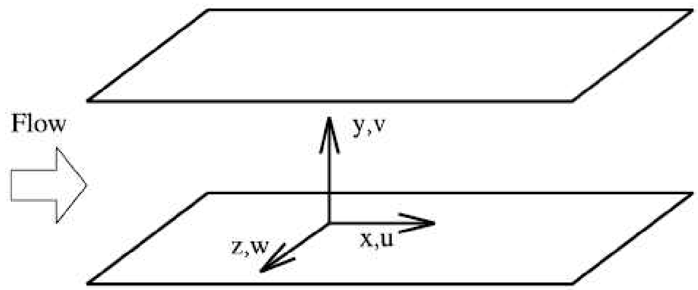
Outline

- **Background & Motivations**
  - Large Eddy Simulation (LES) of turbulent channel flows
  - Numerical methods & main computational kernels
- **Par-LES**: a Parallel Simulation Code for LES based **on parallel scientific libraries for sparse matrix computations**
  - Grid partitioning and parallelism
  - **PSBLAS** for building and applying discrete operators and for sparse linear solvers
  - **MLD2P4** for building and applying algebraic multilevel preconditioners in sparse linear solvers
- **Performance Results**

LES of turbulent channel flows

Bi-periodical plane channel flow



- **N-S eq. (**$Re_\tau = u_\tau\, \delta/\nu$ = 180, 395, 590)
- **Domain sizes**: $2\pi\,\delta \times 2\delta \times \pi\delta$
- **Boundary conditions**: periodic in the streamwise (x) and spanwise directions (z); no-slip at the solid walls (y)
- **Initial condition**: Poiseuille flow with random Gaussian perturbation
- **Pressure forcing term**: assigned along the streamwise direction to set up a constant mass flow rate in the channel
- **LES approach**: FV formulation in which the filtered velocity is based on a *high-order deconvolution top-hat kernel filter*
- **SGS modelling**: *implicit eddy viscosity* due to multidimensional upwind flux discretization

LES of turbulent channel flows (cont'd)

- **Time integration:**
  - time splitting by **Approximate Projection Method** (**APM**)
  - 2nd-order semi-implicit Adams-Bashforth/Crank-Nicolson (AB/CN) scheme
- **Space discretization:**
  - non-uniform grid along y (stretching cosine law)
  - co-located flow variables (center of FVs)
  - multidimensional 3rd-order upwind scheme for convective fluxes
  - 2nd-order central scheme for diffusive fluxes
  - 4th-order formulas for spatial derivatives in inverse deconvolution

A. Aprovitola, F. M. Denaro, *A non-diffusive, divergence-free, Finite Volume-based double projection method on non-staggered grids*, Int. J. Num. Meth. Fluids, 53, 1127-1172, 2007

LES: APM numerical procedure

Helmholtz-Hodge decomposition

$$\tilde{\mathbf{v}}^{n+1} = \mathbf{v}^* - \Delta t \nabla \Phi$$

predictor-corrector approach (velocity field)

where v* is obtained by solving the semi-discrete **deconvolved momentum eq.** neglecting pressure terms

$$\left(A_x^{-1} - \frac{\Delta t}{2\mathrm{Re}_\tau} D_2\right)\mathbf{v}^* = \left(A_x^{-1} + \frac{\Delta t}{2\mathrm{Re}_\tau} D_2\right)\tilde{\mathbf{v}}^n +$$
$$\frac{\Delta t}{2}\left(3\left(\frac{1}{\mathrm{Re}_\tau}(D_1 + D_3)\tilde{\mathbf{v}}^n + \mathbf{f}_{conv}^n\right) - \left(\frac{1}{\mathrm{Re}_\tau}(D_1 + D_3)\tilde{\mathbf{v}}^{n-1} + \mathbf{f}_{conv}^{n-1}\right)\right)$$

with suitable Dirichlet boundary conditions near the walls.

LES: APM numerical procedure (cont'd)

Φ is obtained by solving the so-called **pressure equation**

$$(D_1 + D_2 + D_3)\Phi = \frac{1}{\Delta t \, |\Omega(\mathbf{x})|} \int_{\partial\Omega(\mathbf{x})} \mathbf{v}^* \cdot \mathbf{n} \, dS$$

with Neumann boundary conditions near the walls, ensuring compatibility (a solution exists up to an additive constant)

$$\nabla\Phi = \nabla p + \mathrm{O}(\Delta t)$$

$\nabla\Phi$ is a first order approximation of the pressure gradient

LES: computational kernels

Solution of the deconvolved momentum eq.:

$$\left(A_x^{-1} - \frac{\Delta t}{2\,\mathrm{Re}_\tau} D_2 \right) \mathbf{v}^* = \left(A_x^{-1} + \frac{\Delta t}{2\,\mathrm{Re}_\tau} D_2 \right) \tilde{\mathbf{v}}^n$$

$$+ \frac{\Delta t}{2} \left(3 \left(\frac{1}{\mathrm{Re}_\tau} (D_1 + D_3) \tilde{\mathbf{v}}^n + \mathbf{f}_{conv}^n \right) - \left(\frac{1}{\mathrm{Re}_\tau} (D_1 + D_3) \tilde{\mathbf{v}}^{n-1} + \mathbf{f}_{conv}^{n-1} \right) \right)$$

! $N=N_x \, x N_y \, x \, N_z$ total number of grid cells

1. ***compute** discrete inverse deconvolution by 4th-order scheme*

   $A_x^{-1} \rightarrow \mathbf{A} \in \Re^{N \times N}$

2. ***compute** discrete diffusive operators by 2nd-order scheme*

   $D_1, D_2, D_3 \rightarrow \mathbf{D}_i \in \Re^{N \times N}$

⇒ **Build sparse matrices independent of time-step**

LES: computational kernels (cont'd)

Solution of the deconvolved momentum eq. (cont'd):

! $N=N_x \, x N_y \, x \, N_z$ total number of grid cells

3. compute *discrete convective fluxes by multidimensional 3th-order up-wind scheme*

$\mathbf{f}_{conv}^{n}, \mathbf{f}_{conv}^{n-1}$ ➡ $\mathbf{q}_i^{n} = \alpha \mathbf{u}_i^{n}, \; \mathbf{q}_i^{n-1} = \alpha \mathbf{u}_i^{n-1} \qquad i = 1,2,3$ ⇨ **vectors updates**

4. build *rhs and coefficient matrix of the* **velocity systems**

$$\mathbf{M}\mathbf{v}_i^* = \mathbf{w}_i \quad \textit{with} \quad \mathbf{v}^* = (\mathbf{v}_i^*)_{i=1,2,3}$$

$$\mathbf{M} = \mathbf{A} - \beta \cdot \mathbf{D}_2$$

$$\mathbf{w}_i = (\mathbf{A} + \beta \cdot \mathbf{D}_2)\tilde{\mathbf{v}}_i^{\,n} +$$

$$+ \tau\left(3\left(\lambda \cdot (\mathbf{D}_1 + \mathbf{D}_3)\tilde{\mathbf{v}}_i^{\,n} + \mathbf{q}_i^{n}\right) - \left(\lambda(\mathbf{D}_1 + \mathbf{D}_3)\tilde{\mathbf{v}}_i^{\,n-1} + \mathbf{q}_i^{n-1}\right)\right)$$

⇨ **matrices updates/matrix-vector products/vector updates**

N.B. matrices independent of time-step

LES: computational kernels (cont'd)

Solution of pressure equation

$$(D_1 + D_2 + D_3)\Phi = \frac{1}{\Delta t \, |\Omega(\mathbf{x})|} \int_{\partial\Omega(\mathbf{x})} \mathbf{v}^* \cdot \mathbf{n} \, dS$$

! $N=N_x \, x N_y \, x \, N_z$ total number of grid cells

*1. **build** rhs and coefficient matrix of the sparse linear system*

$$\mathbf{D}\,\varphi = \mathbf{s}$$

$$\mathbf{D} = \mathbf{D}_1 + \mathbf{D}_2 + \mathbf{D}_3 \in \Re^{NxN}$$
$$\mathbf{s} \in \Re^{N}$$

matrices updates/vector update

N.B. matrix independent of time-step

LES: time-marching procedure

APM procedure

Build sparse matrices/vectors → **Sparse Matrix Management** (allocate, build, update)

! Nsteps = total number of time steps

for *n = 1, Nsteps* ***do***

1. ***compute*** *convective fluxes*
2. ***compute*** *diffusive fluxes*
3. ***compute*** *deconvolved velocity*

→ **Sparse BLAS** (matrix-vector prod.,vector up.)

4. ***solve*** *deconvolved momentum eq.*
5. ***solve*** *pressure eq.*

→ **Solution of sparse linear systems** (~75% of total cost)

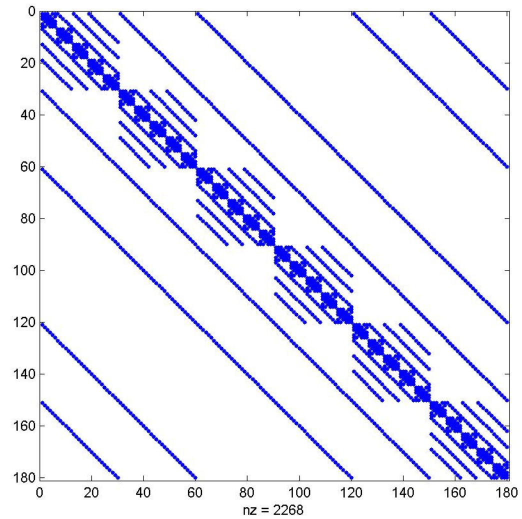
6. ***update*** *velocity*

endfor

Number of time steps and dimensions of matrices/vectors increasing with Reynolds number

LES: sparse linear solvers

Solution of velocity systems:



$$\mathbf{M}\mathbf{v}_i^* = \mathbf{w}_i \quad \textit{with} \quad \mathbf{v}^* = (\mathbf{v}_i^*)_{i=1,2,3}$$

Three linear systems whose matrix is:

✓large and sparse
✓unsymmetric with symmetric sparsity pattern
✓diagonally dominant

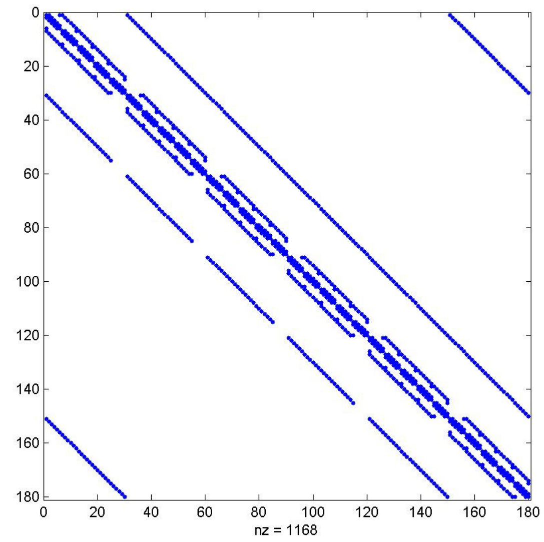
GMRES with point-Jacobi preconditioner

accounts for ~ 40% of the total run-time

LES: sparse linear solvers (cont'd)

Solution of pressure system:

$$\mathbf{D}\,\varphi = \mathbf{s}$$



Singular, but compatible linear system, whose matrix is

✓large & sparse
✓unsymmetric with symmetric sparsity pattern
✓condition number rapidly increasing for decreasing grid sizes

GMRES with Multilevel DD Preconditioners

accounts for ~ 35% of the total run-time

Par-LES

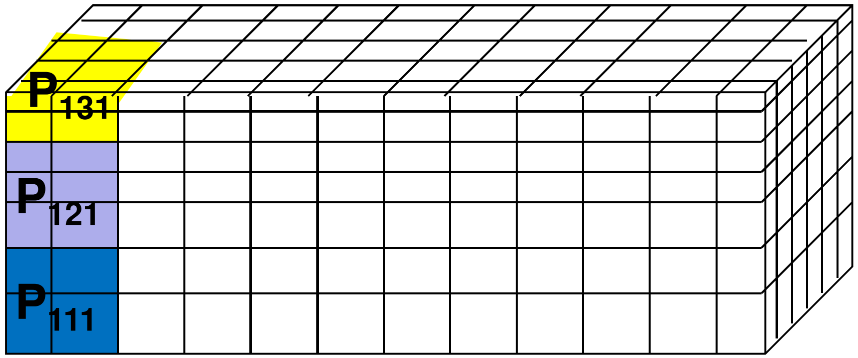
a parallel code for LES

based on portable, efficient and reliable **scientific libraries for parallel sparse matrix computations**

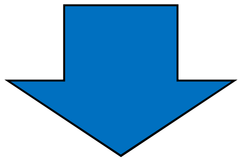
- Simplicity in changing numerical methods/solvers (modularity, flexibility)
- Parallelism encapsulated in library routines and support for distributed data structures creation/management (rapid and "low-cost" introduction of parallelism)
- Up-to-date parallel algorithms and standard base software (efficiency, portability,robustness)

Par-LES: basic choice for parallelism

Data parallelism based on 3D decomposition of computational grid

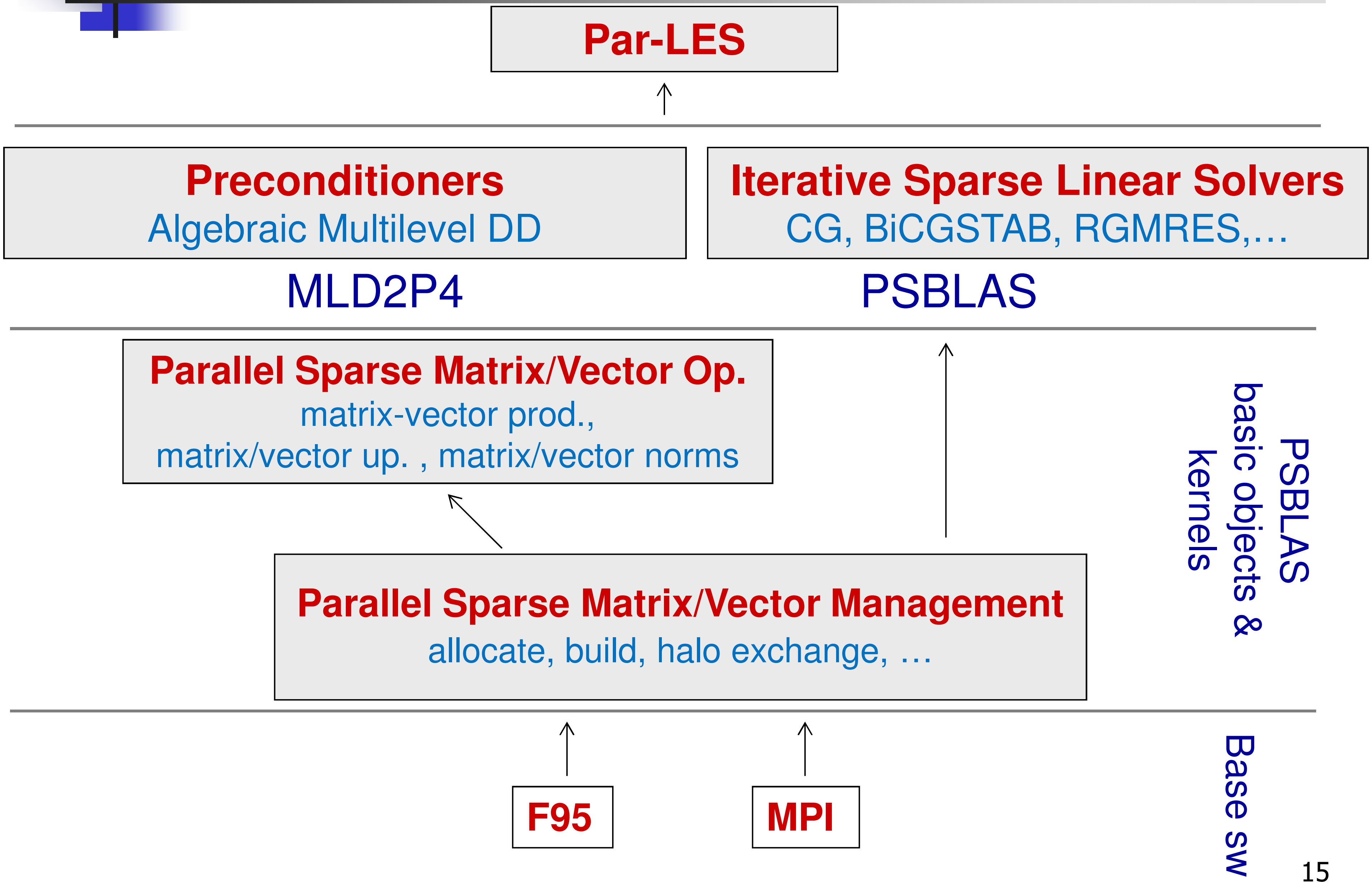


- ✓Processors are connected in a 3D Cartesian virtual topology
- ✓Every processor owns a 3D sub-block of computational grid, i.e. a block of consecutive rows of the matrices/vectors
- ✓Every processor locally computes on its internal points (*volume of sub-block*)
- ✓Nearest-neighbor processors communicate some layers of "halo" points (surface of sub-block)



Surface to volume effect, i.e. minimize T_{com}/T_{calc}

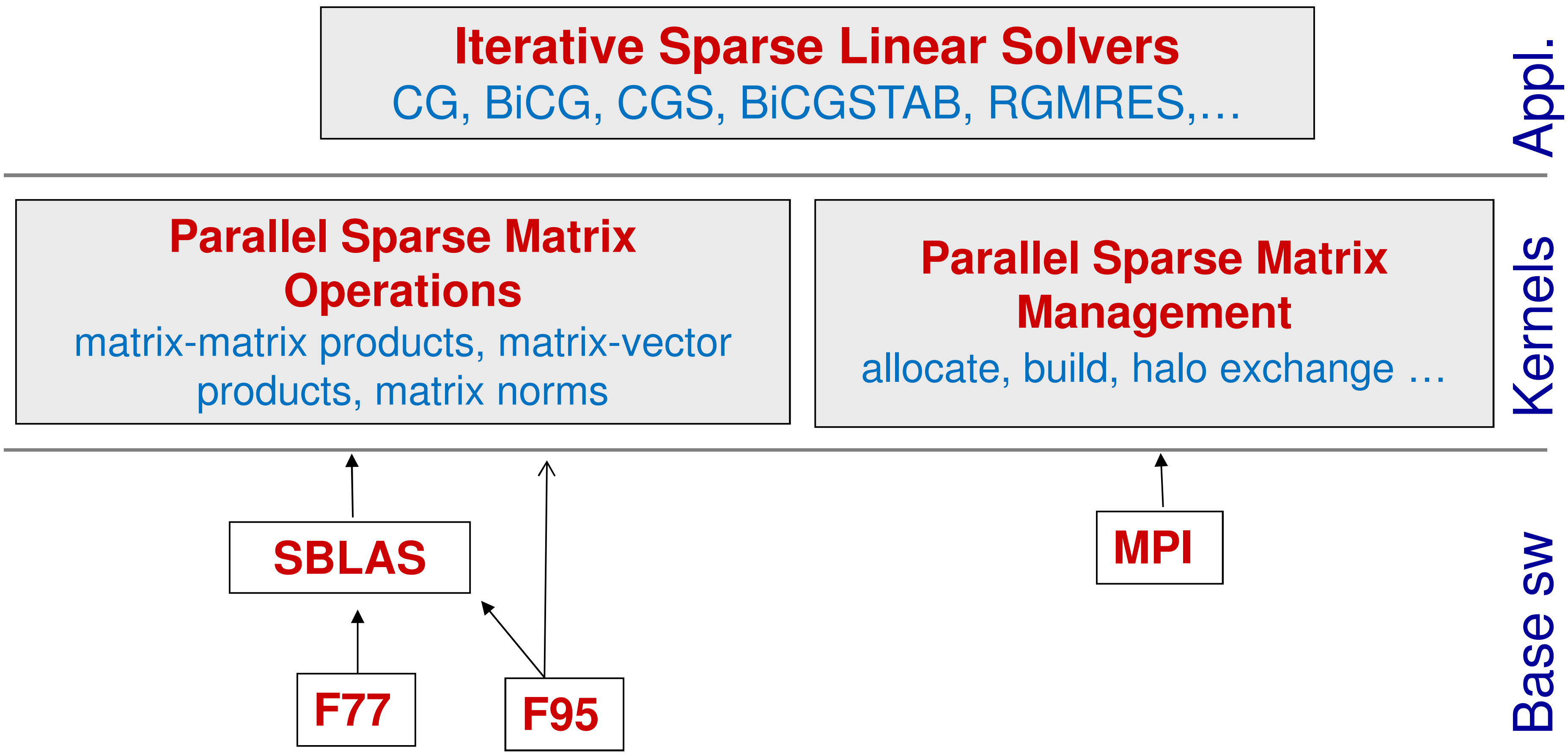
Par-LES: Software Architecture



PSBLAS (Filippone et al., www.ce.uniroma2.it/psblas/)

Parallel Sparse BLAS rel. 2.4

Basic Linear Algebra Operations with Sparse Matrices
on MIMD Architectures



Multilevel DD preconditioners

Domain Decomposition (DD) preconditioners:

- divide the PDE domain (the matrix) into subdomains (submatrices)
- apply a "local preconditioning" in each subdomain
- build the global preconditioner from the local ones

Additive Schwarz preconditioners – pros & cons:

- naturally fit in a parallel environment → good implementation scalability
- # iterations of the preconditioned solver grows with # subdomains
  → poor algorithmic scalability

Use of multiple level corrections to obtain optimal preconditioners
(# iterations bounded independently of grid size and subdom. diameter)

MLD2P4 (www.mld2p4.it)

Multi-**L**evel **D**omain **D**ecomposition
Parallel **P**reconditioners **P**ackage based on **PSBLAS**

mld_precbld(A,M,…)
A, distributed sparse matrix (input)
M, distributed sparse preconditioner (output)

mld_precaply(M,x,y,…)
M, distributed sparse preconditioner (input)
x,y, distributed vectors (input/output)

Diagonal
Block-Jacobi
Additive Schwarz with arbitrary overlap
Algebraic multi-level Schwarz based on aggregation

PSBLAS 2.0
extended version of PSBLAS 1.0

P. D'Ambra, D. di Serafino, S. Filippone, *MLD2P4: a Package of Parallel Algebraic Multilevel Domain Decomposition Preconditioners in Fortran 95*, ACM Transactions on Mathematical Software, Vol. 37, N. 3, 2010.

Preconditioners available in MLD2P4

Any combination of the following components

- Base (1-lev) preconditioner (smoothers):
  point-Jacobi, block-Jacobi, additive Schwarz (AS, RAS, ASH) with
  LU (UMFPACK) or ILU fact. (ILU(p), MILU(p), ILU(t,p)) of the blocks
- Multilevel type:
  additive or multiplicative, with pre-, post- or two-side smoothing
- Coarsening strategy:
  decoupled classical or unsymmetric smoothed aggregation
- Coarsest-level matrix:
  distributed or replicated
- Coarsest-matrix solver:
  ILU, sparse LU (UMFPACK, SuperLU, SuperLU_Dist), block-Jacobi with
  ILU or LU on the blocks, pont-Jacobi

Par-LES: Test Case

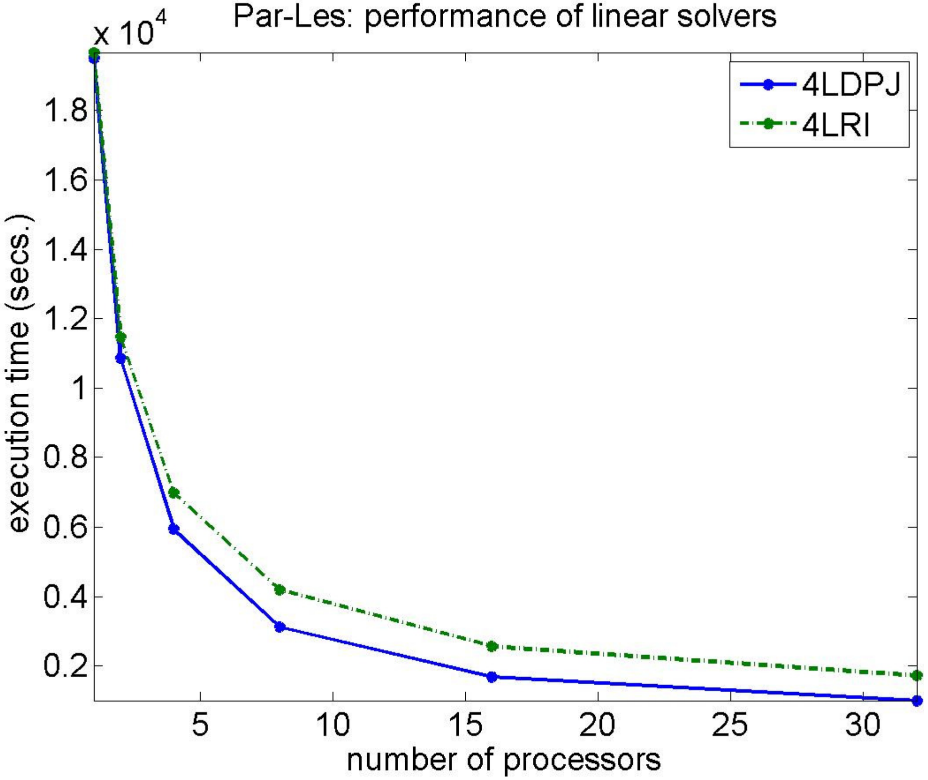
- $Re_\tau = 590$
- Number of grid cells: 48x100x48
  (providing a resolved boundary layer with minimum cell size $\Delta y+ = 0.145$)
- $\Delta t = 10^{-5}$ (estimated on the base of linear stability constraints)
- Matrices Dimension: N=228096
  - Nonzeros for velocity 2960640, Nonzeros for pressure 1589902
- Preconditioners for pressure system:
  - 4-lev V cycle, with RAS(1) as smoother, replicated coarse matrix: 4 sweeps of Block Jacobi with ILU(0) on diagonal blocks **(4LRI)**
  - 4-lev V cycle, with Block Jacobi as smoother, distributed coarse matrix: 4 sweeps of Point Jacobi **(4LDPJ)**
- Stopping criterion for linear solvers:: $\| r_k \| / \| r_0 \| \leq 10^{-7}$ or maxiter

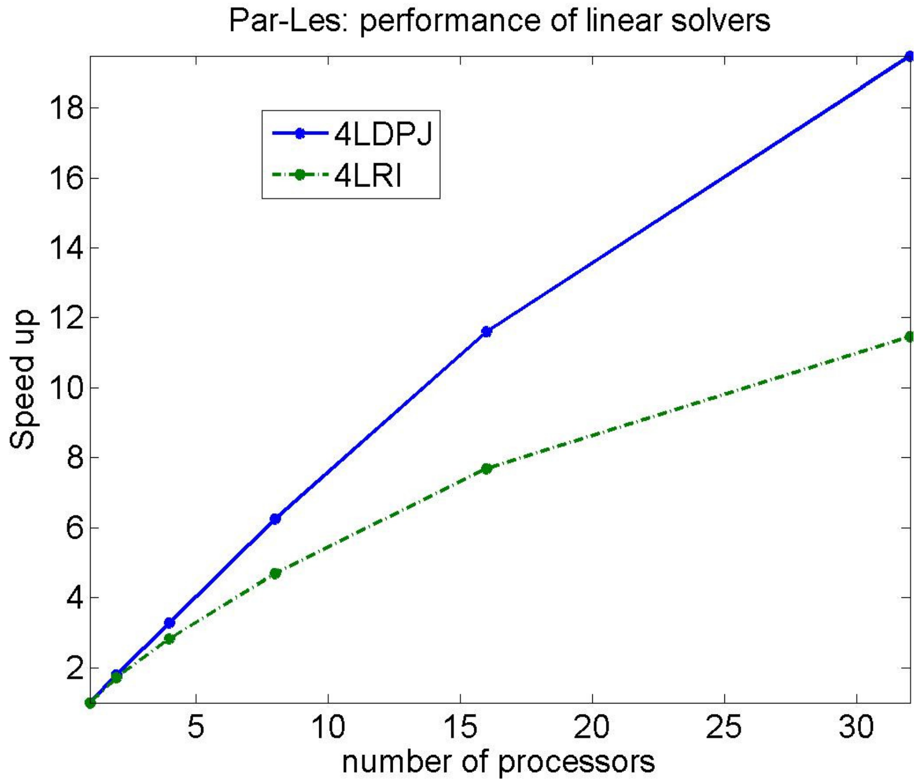
Par-LES: computational environment

HP XC 6000 Linux cluster

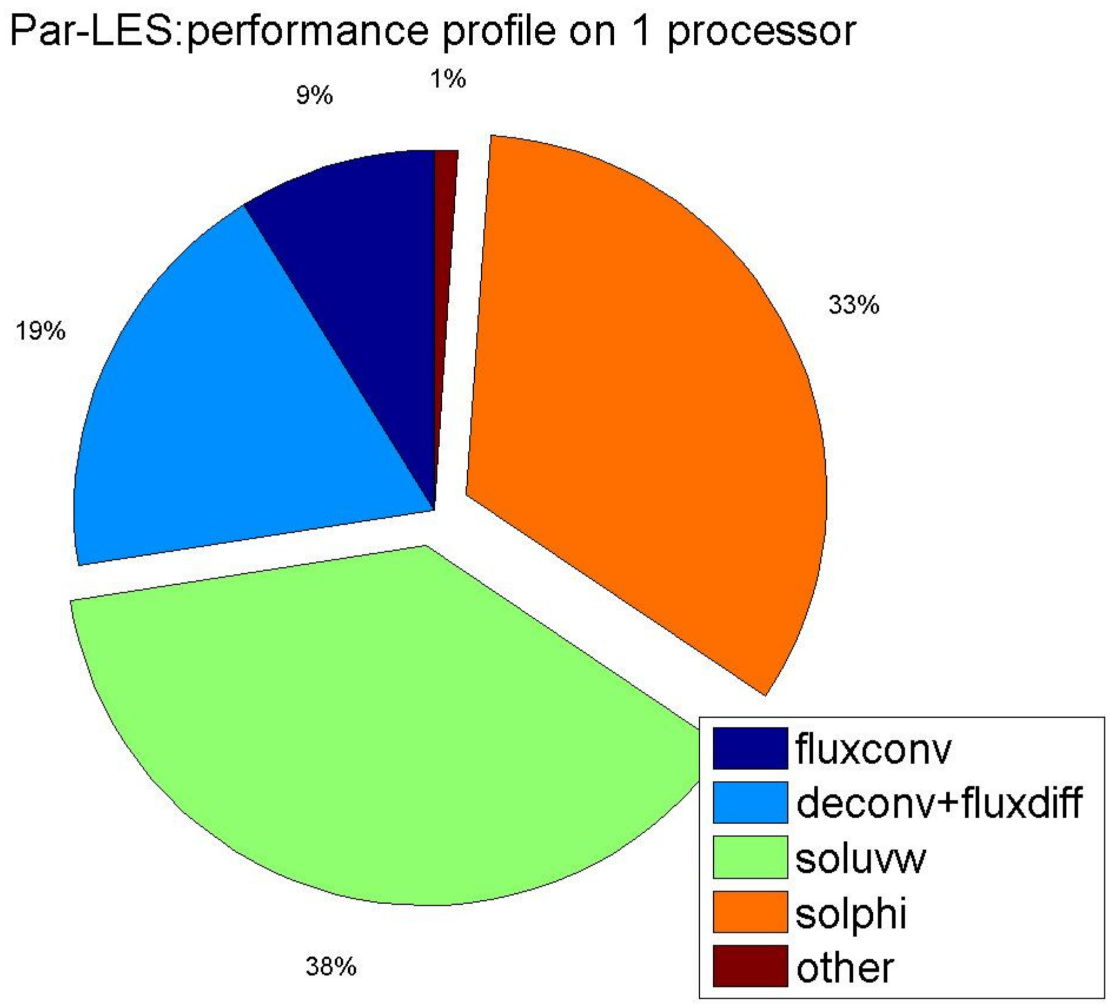
- 64 Intel Itanium 2 Madison (1.4 GHz) bi-processor nodes with 4 GB of RAM
- Quadrics QsNetII Elan 4 interconnection network (900 MB/sec. of bandwidth and 5μsec. of latency)
- HP Linux for High Performance Computing, based on Red Hat Enterprise Linux AS 3 with Kernel 2.4.21
- GNU 4.6 compilers
- HP MPI implementation
- BLAS implementation provided by ATLAS 3.6.0
- PSBLAS 2.4

Par-LES: performance results (2000 time steps)

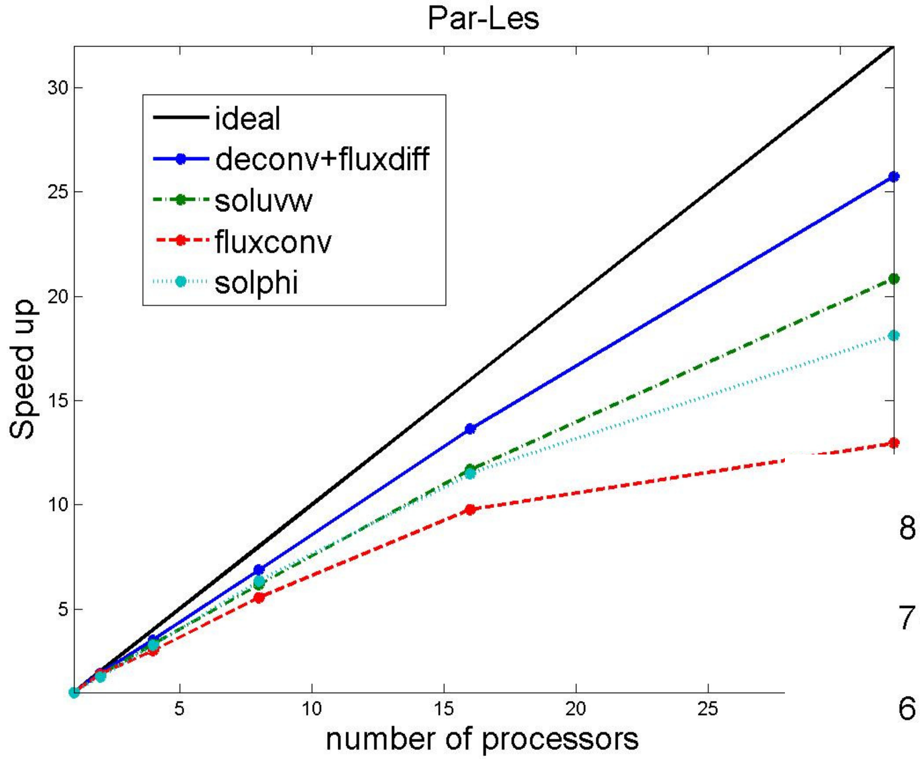


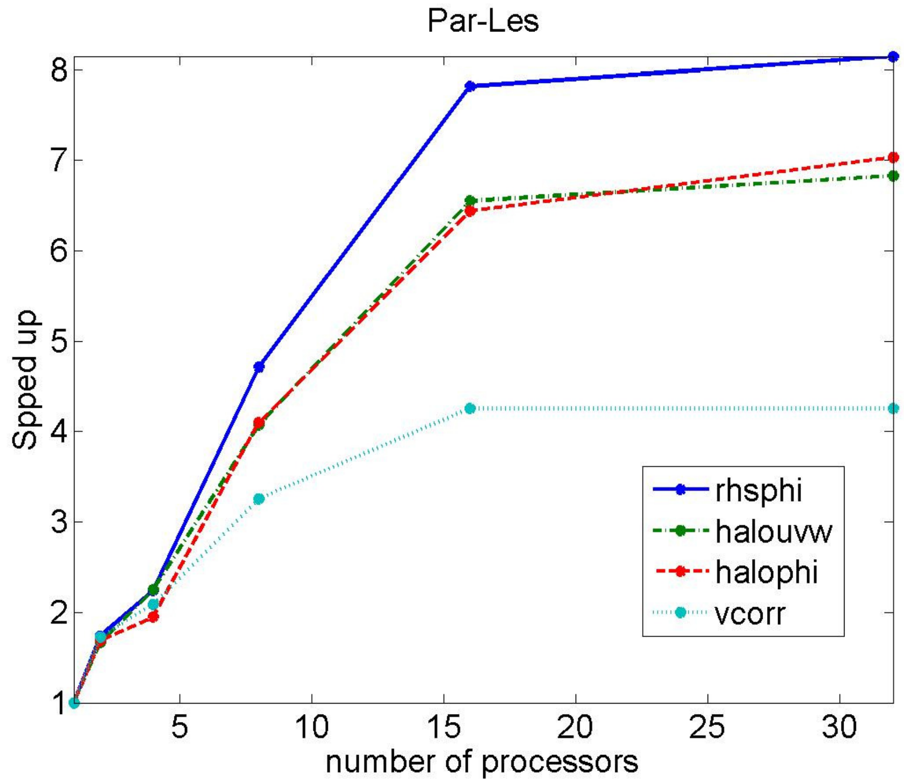


Par-LES: performance results (4LDPJ-2000 time steps)

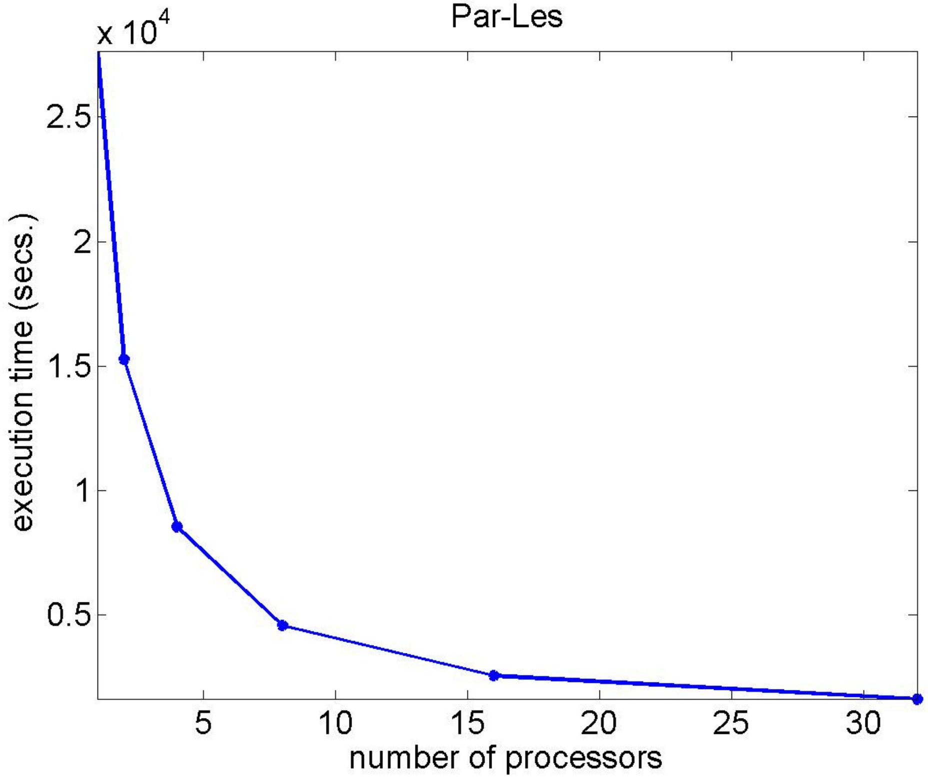


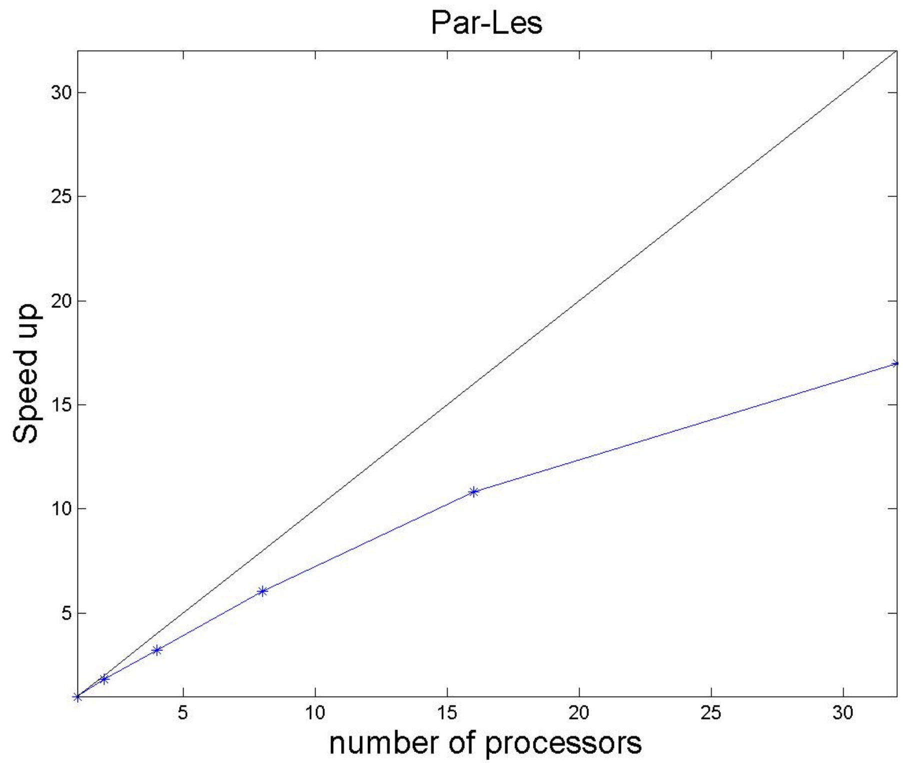
Par-LES: performance results (4LDPJ-2000 time steps)





Par-LES: performance results (4LDPJ-2000 time steps)





Concluding remarks

- **Par-LES** shows good **strong scalability** for medium size Reynolds numbers
- **Par-LES is based on portable and reliable** open-source **parallel scientific libraries** based on MPI, thus it can be run on different architectures on which MPI is available.
- **Many variants of linear solvers and preconditioners can be tested** by changing only input parameters
- **Improvements or extensions to PSBLAS/MLD2P4 libraries** (shift through many-core/GPU architectures) **will be available to Par-LES with no effort**

Thank you for your attention