Introduction to the SBLI code

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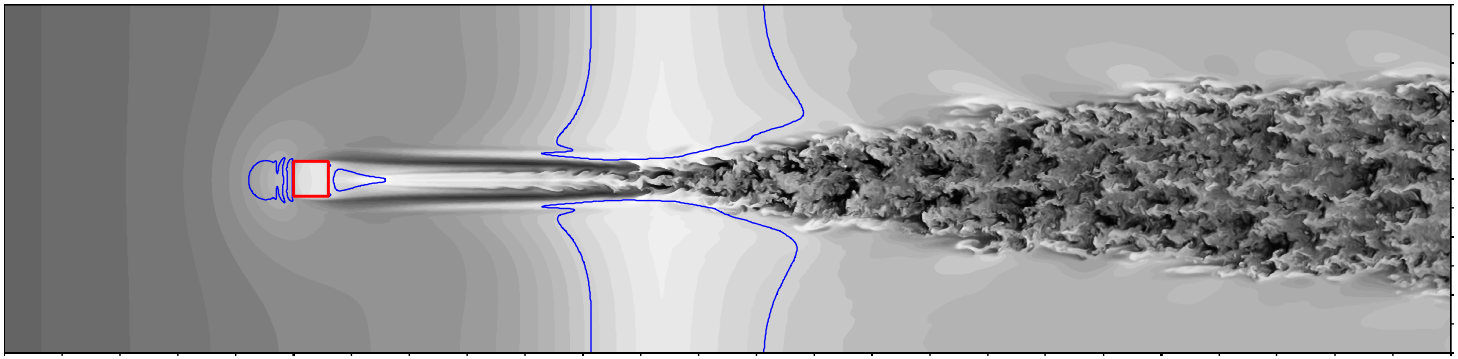
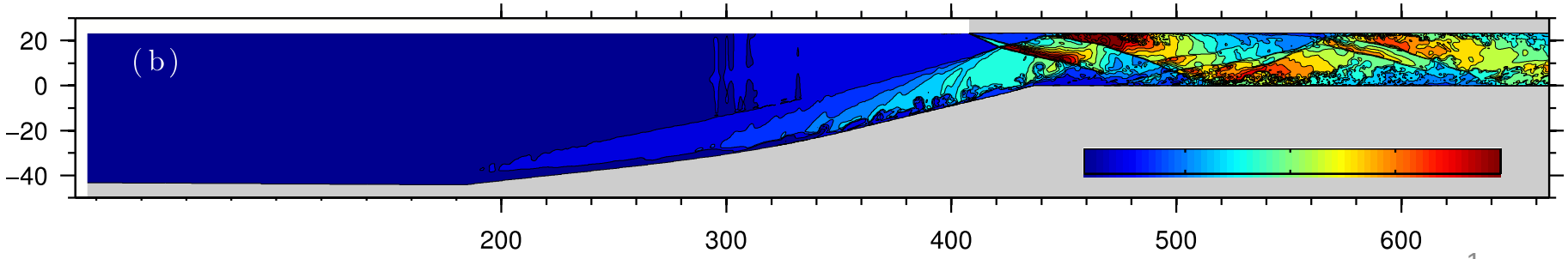




Outline

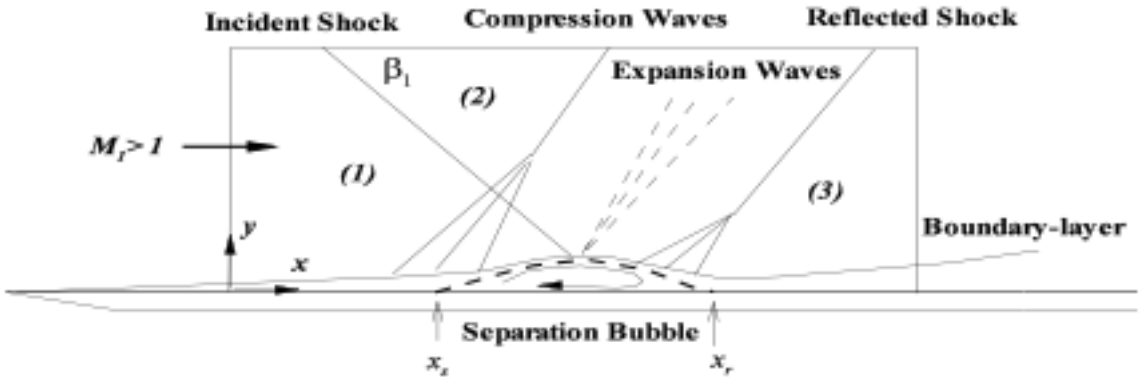
- Overview of the numerical algorithms
- Review of recent code re-engineering
- Examples of current numerical investigations
- Code design and structure
- Introduction to HiPSTAR – new code building partly on SBLI structure

Numerics overview

- Compressible Navier-Stokes solver (Fortran 95+)
- 4^{th} order central differences (5-point stencil)
- 3^{rd} order explicit Runge-Kutta (RK3 and RK4) time advance
- Stability improved via an entropy splitting approach
- Characteristic BCs to avoid wave reflections
- Shock capturing with TVD
- Implicit 6^{th} order filter (7-point stencil)
- Multi-block capabilities
- Inter- and intra-block parallelism using MPI (in-house library)

Previous re-engineering project[1]

- Unifications of different code versions: Multi-block, LES, Airfoil simulations (C-grid), fully 3D code version (3D curvilinear grids)
- Update to Fortran 95+ standard
- Development of a validation suite including:
  - Shock boundary-layer/interactions



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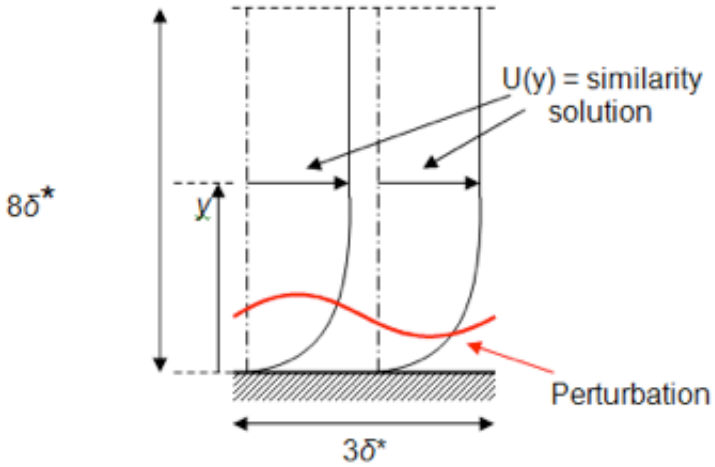

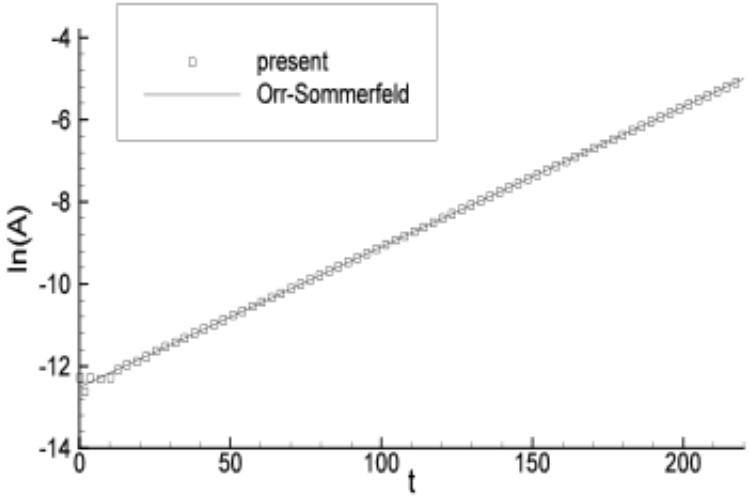

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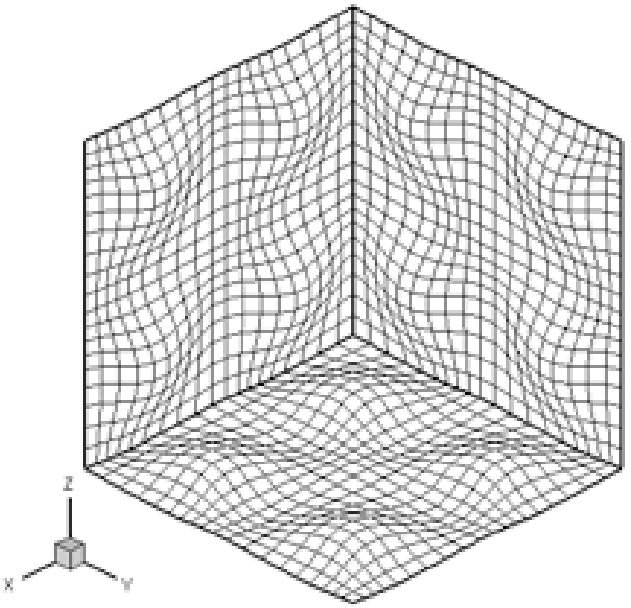

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  - 3D curvilinear capability
- Scalability tests
  - up to 1024 processors in 2009
  - up to 200,000 by Mike Ashworth (Daresbury Lab.)

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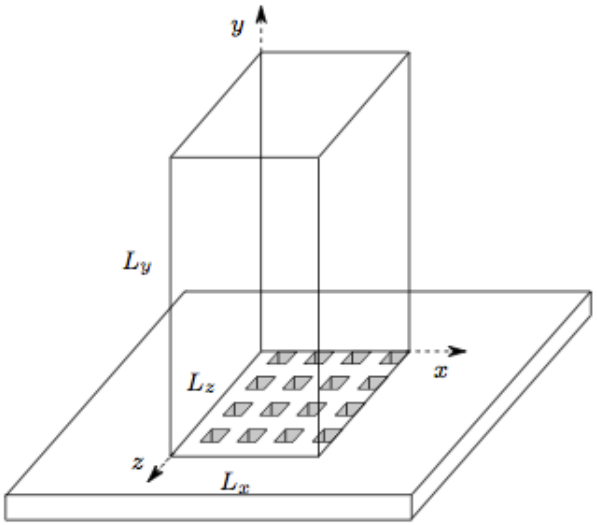
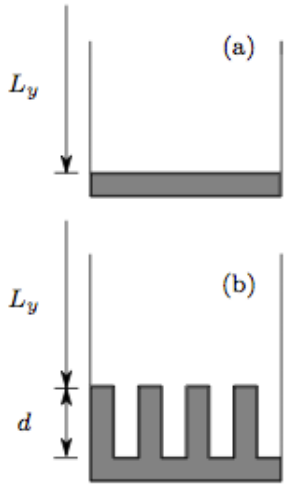
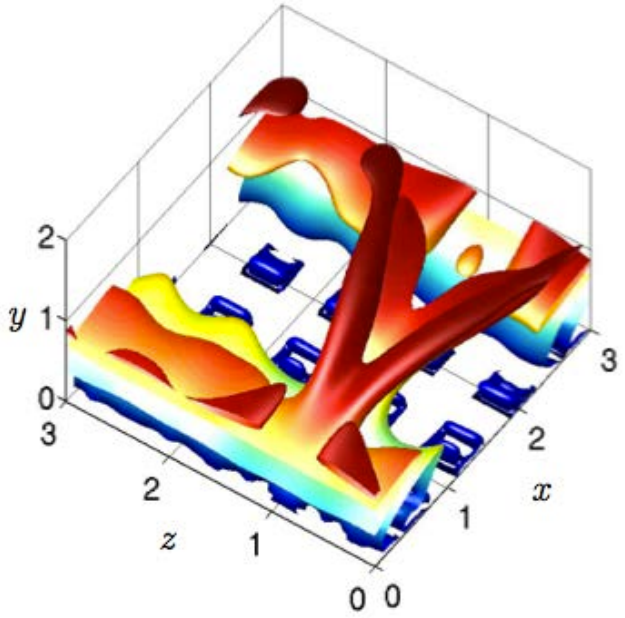
Current research examples

a) Boundary-layer instability over a porous surface



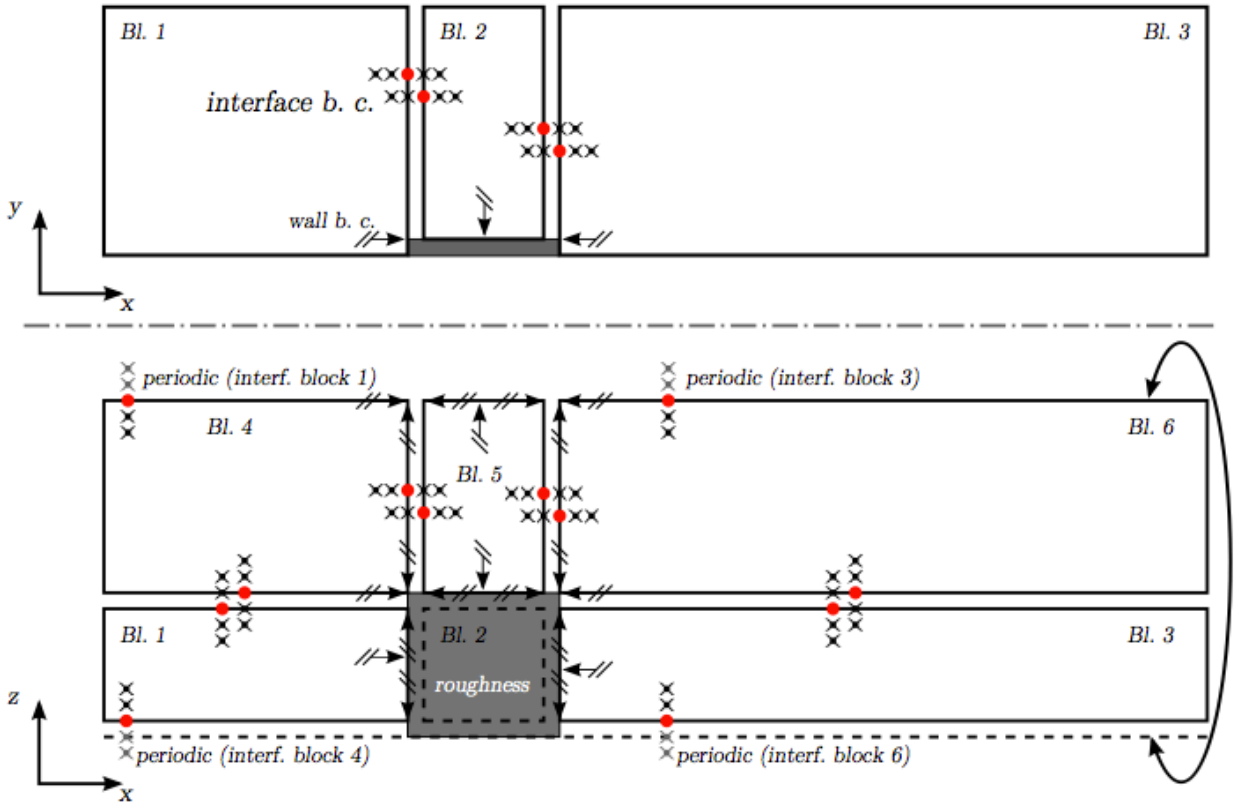




- 64 blocks
- Approximately 150,000 points per block

Current research examples

b) Roughness-induced transition to turbulence



- 6 blocks
- 156 million points in block 6, 2 million in block 2

Current research examples

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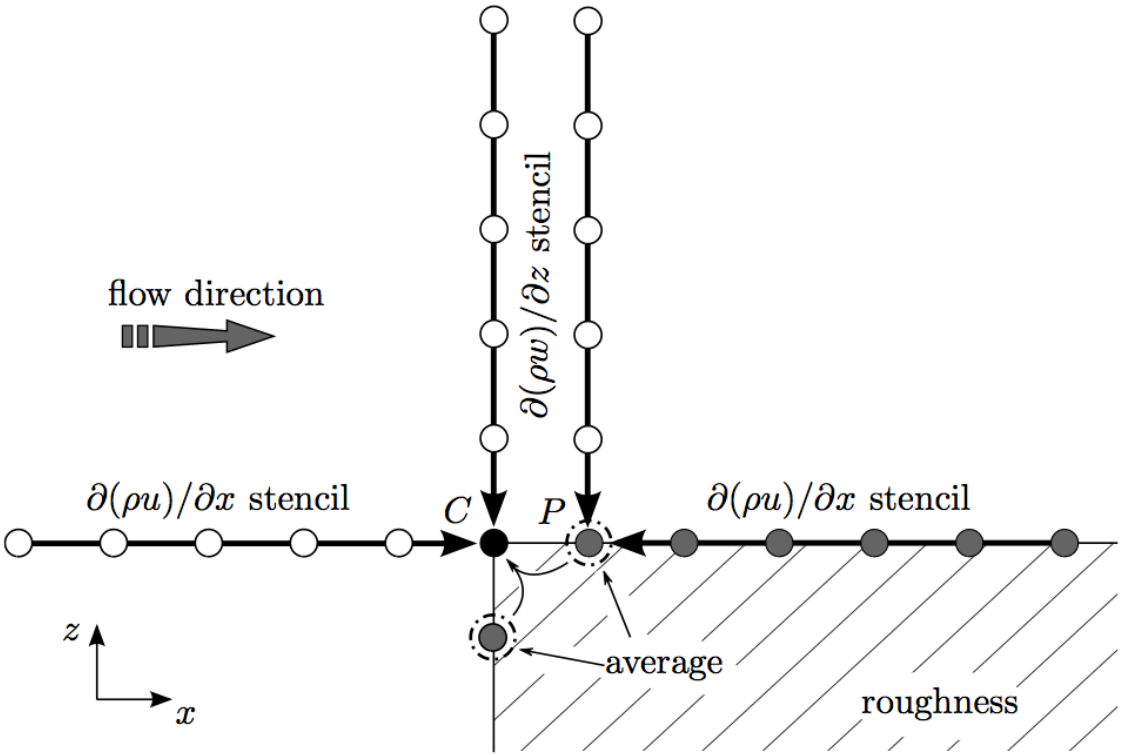

- 6 blocks
- 156 million points in block 6, 2 million in block 2
- Special treatment of density at edges

Code design

1. Number and size of blocks: 1-64 with 100,000 to 200 M points
2. Block connectivity: matching nodes
3. FD stecil: 5 points, 2 halos (central diff), 7 points, 3 halos (filter), 6-point stencil for one-sided scheme
4. Time-marching: explicit
5. Language: FORTRAN 95 - 2000
6. Parallelism: MPI
7. Inter-block communications: own “swap” routines (more later)
8. Mesh refinement: No
9. Data per grid-point: 70 numbers (work arrays and metrics)
10. Parallel I/O: MPI I/O (seems problematic for large arrays)
11. Viz. during parallel exec: No, but might be worth looking at
12. Other notes: grid and multi-block interfaces loaded by one proc and broadcast to the rest

Code structure

```
INIT (allocate arrays, read grids and block interf, set communicators, etc…)
do t = tin, tend
    do i = 1, RKsteps
        call SWAP
        call RHS  ! most of the effort due to work array multiplication
        call BC
    end do
    if(filter) call SWAP, call FILTER
    if(TVD) call SWAP, call TVD
    if(writeflag) call WRITE_Q
end do
end program
```

Swap routines for inter-block comm.

```
l = 0
do intf = 1, intf_num
   intf_start(intf) = l+1
   do n = intf_start, intf_end
      l = l+1
      qout(l) = q(n) ! pack halo data for all interfaces into contiguous array
   end do
end do
! Communicate
do intf = 1, intf_num
   intfproc = intf_proc(intf) ! interface processor for this interface (set in init stages)
   l = intf_start(intf)
   call MPI_isend(qo(l), count, type, intfproc, intf_intercomm(intf), request, ierr)
   call MPI_irecv(qin (l), count, type, intfproc, intf_intercomm(intf), request, ierr)
end do
```

Typical RHS structure

```
! Viscosity calculation
do k = 1-zhalo:nz+zhalo
   do j = 1-yhalo:ny+yhalo
      do i = 1-xhalo:nx+xhalo
         wx(i,j,k,1-4) = q(i,j,k,1-4) ! rho, rho*u, rho*v, rho*w
         wx(i,j,k,7) = q(i,j,k,5) ! rho*E
         q(i,j,k,2-4) = q(i,j,k,2-4)/q(i,j,k,1) ! u, v and w
         wx(i,j,k,5) = ct*wx(i,j,k,7)/wx(i,j,k,1)-0.5*(q(i,j,k,2)*q(i,j,k,2)
                                                      +q(i,j,k,3)*q(i,j,k,3)
                                                      +q(i,j,k,4)*q(i,j,k,4)) ! Temperature
         wx(i,j,k,17) = reinv*(wx(i,j,k,5)*sqrt(wx(i,j,k,5))*
                              (1+T1/T2)/(wx(i,j,k,5)+T1/T2) ! Viscosity
      end do
   end do
end do
```