Implementation of a compressible-flow simulation code in the D programming language

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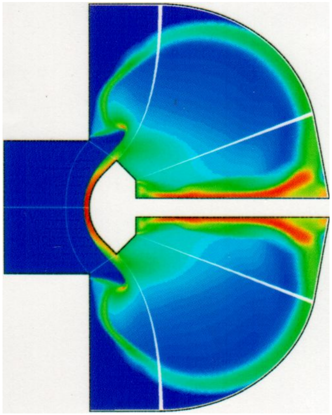
History

Eilmer4, formulation

Examples

Eilmer in a nutshell



- Eulerian/Lagrangian description of the flow (finite-volume, axisymmetric or 3D)
- Transient, time-accurate
- Shock capturing
- Multiple-block, structured and unstructured grids
- Parallel computation on a cluster computer, using MPI in Eilmer2,3
- High-temperature thermochemistry and dense-gas module

Origins

- in the late 1980s, the state of the art for scramjet simulations involving reactive flow was JP Drummond *SPARK* code
- Flow solver component based on Bob McCormack's (1969) finite-difference shock-capturing technique.
- All configuration hard-coded into the Fortran source code and compiled to run on a Cray supercomputer.
- In the 1980s, a new CFD technology (upwind flux) was being developed by the applied mathematics people and parallel computing environments were being developed by the computer science people (cluster computers).
- Dec 1990: following a CFD lesson on the chalk-board from Bob Walters and Bernard Grossman, *cns4u* was started with the intention to be like SPARK but with new technology

Development of Eilmer

- 1993 built *sm3d*, a space-marching code for 3D scramjet flows
- 1995 through 1999: the postgrad years expanded scope of experimentation and application
- 1996: code reformulation around fluxes (frequent discussions with Mike Macrossan); all code still in C with a preprocessor having a little command interpreter built in.
- 1997: discovered scripting languages Tcl and Python
- May 2003: *scriptit.tcl* provided fully programmable environment for simulation-preparation.
- Aug 2004: *Elmer* began as a hybrid code using Python and C.
- Jun 2005: rewrite of *Elmer(2)* in C alone so that Andrew Denman could get on with his thesis
- Jul 2006: rewrite *Elmer2* in C++ and, in 2008, call it *Eilmer3*. The class-based implementation was easier to extend and maintain.

Eilmer4 – Let's do it right, again.

Fred Brooks, in the "Mythical Man-Month: Essays on software engineering"

> *Sooner or later the first system is finished, and the architect, with firm confidence and a demonstrated mastery of the class of systems, is ready to build a second system. ...*
> *This second is the most dangerous system a man ever designs. ...*
> *The general tendency is to over-design the second system, using all the ideas and frills that were cautiously sidetracked on the first one.*

We're OK, this is not our second system.
cns4u, mbcns, mbcns2, Elmer, Elmer2, Eilmer3 ... Eilmer4.

Mathematical gas dynamics (in differential form)

Conservation of mass:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot \rho \mathbf{u} = 0 \tag{1}$$

Conservation of species mass:

$$\frac{\partial}{\partial t}\rho_i + \nabla \cdot \rho_i \mathbf{u} = -\left(\nabla \cdot \mathbf{J}_i\right) + \dot{\omega}_i \tag{2}$$

Conservation of momentum:

$$\frac{\partial}{\partial t}\rho \mathbf{u} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla p - \nabla \cdot \left\{-\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\dagger}) + \tfrac{2}{3}\mu(\nabla \cdot \mathbf{u})\boldsymbol{\delta}\right\} \tag{3}$$

Conservation of total energy:

$$\begin{aligned}\frac{\partial}{\partial t}\rho E + \nabla \cdot (e + \frac{p}{\rho})\mathbf{u} &= \nabla \cdot [k\nabla T + \sum_{s=1}^{N_v} k_{v,s}\nabla T_{v,s}] + \nabla \cdot \left[\sum_{i=1}^{N_s} h_i \mathbf{J}_i\right] \\ &- \left(\nabla \cdot \left[\left\{-\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\dagger}) + \tfrac{2}{3}\mu(\nabla \cdot \mathbf{u})\boldsymbol{\delta}\right\} \cdot \mathbf{u}\right]\right) - Q_{\text{rad}}\end{aligned} \tag{4}$$

Conservation of vibrational energy:

$$\frac{\partial}{\partial t}\rho_i e_{v,i} + \nabla \cdot \rho_i e_{v,i}\mathbf{u} = \nabla \cdot [k_{v,i}\nabla T_{v,i}] - \nabla \cdot e_{v,i}\mathbf{J}_i + Q_{T-V_i} + Q_{V-V_i} + Q_{\text{Chem}-V_i} - Q_{\text{rad}_i} \tag{5}$$

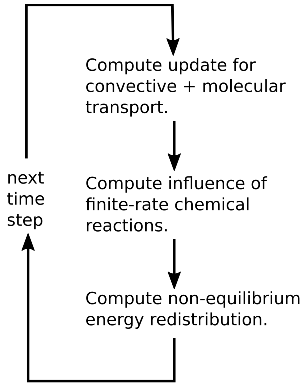
More maths...

Thermodynamic model of the gas...
Finite-rate chemical kinetics...
Radiation energy exchange...
Boundary conditions...
Features:

- 3D from the beginning, 2D as a special case
- structured- and unstructured-meshes for complex geometries
- refined thermochemistry
- moving meshes (Jason Qin and Kyle Damm)
- simplified and generalized boundary conditions
- coupled heat transfer
- shared-memory parallelism for multicore workstation use
- block-marching for speed (nenzfr and nozzle design)

Software implementation

- D language data storage and solver, with embedded Lua interpreters for preprocessing, user-controlled run-time configuration in boundary conditions and source terms and thermochemical configuration.


Compute update for convective + molecular transport.
Compute influence of finite-rate chemical reactions.
Compute non-equilibrium energy redistribution.
next time step

```
for s=1 to n do:
    clear flux data
    apply pre-reconstruction action
    detect shock points
    reconstruct flow data at cell interfaces
    compute convective fluxes
    apply pre-spatial-derivative action
    compute spatial derivatves
    apply post-differential flux action
    add source terms if any
    compute time derivatives of conserved quantities
    update cell-average conserved quantities for stage s
    decode conserved quantities to all flow quantities
```

Collecting the low-hanging fruit of parallelism

```
// Determine the allowable time step -- serial version.
double dt_allow = 1.0e9;
foreach (myblk; gasBlocks) {
    if (!myblk.active) continue;
    double local_dt_allow = myblk.determine_time_step_size(dt_global);
    dt_allow = min(dt_allow, local_dt_allow);
}



// Determine the allowable time step -- parallel version.
shared double dt_allow = 1.0e9;
foreach (myblk; parallel(gasBlocks,1)) {
    if (!myblk.active) continue;
    double local_dt_allow = myblk.determine_time_step_size(dt_global);
    dt_allow = min(dt_allow, local_dt_allow);
}
```

Notes:

- Need to keep most data thread local.
- D Compiler expands “parallel” into code that hands out tasks to the default ThreadPool.

Verification and Validation Examples

Verification:

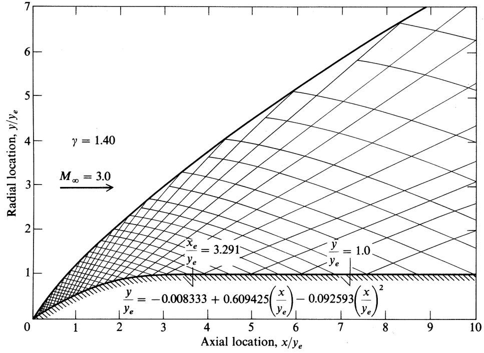
- Are we solving the equations correctly?
- Compare with numerical solutions from other codes.
- Manufactured solution that we must match (using special source terms and BCs).

Validation:

- Are we solving the correct gas-dynamic equations?
- Compare with experimental measurements.

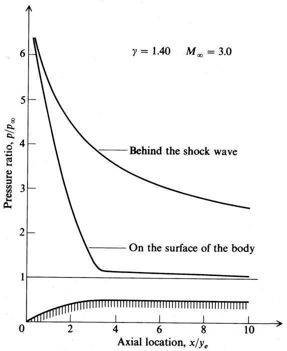
Example 1: sharp-nosed projectile

- Original Zucrow & Hoffman; also Anderson's Hypersonics text
- Shape of surface defined by polynomial equation
- Can compare numerical solutions



Radial location, y/y_e
$\gamma = 1.40$
$M_\infty = 3.0$
$\frac{x_e}{y_e} = 3.291$
$\frac{y}{y_e} = 1.0$
$\frac{y}{y_e} = -0.008333 + 0.609425\left(\frac{x}{y_e}\right) - 0.092593\left(\frac{x}{y_e}\right)^2$
Axial location, x/y_e

FIGURE 5.5
A typical characteristics mesh. (*From Zucrow and Hoffman, Ref. 53.*)



Input script – gas model and flow

```lua
-- sharp.lua
config.title = "Mach 3 flow over a sharp 2D body"
print(config.title)

nsp, nmodes = setGasModel('ideal-air-gas-model.lua')
print("GasModel set to ideal air. nsp= ", nsp, " nmodes= ", nmodes)
initial = FlowState:new{p=5955.0, T=304.0, velx=0.0, vely=0.0}
inflow = FlowState:new{p=95.84e3, T=1103.0, velx=2000.0, vely=0.0}

```

Notes:

- user's input script is Lua source code
- arguments to function calls delimited by ()
- tables delimited by {}
- object model by convention as described in Ierusalimschy's book "Programming in Lua"

Input script – user-defined functions

```
-- Geometry of flow domain.
function y(x)
   -- (x,y)-space path for x>=0
   if x <= 3.291 then
      return -0.008333 + 0.609425*x - 0.092593*x*x
   else
      return 1.0
   end
end

function xypath(t)
   -- Parametric path with 0<=t<=1.
   local x = 10.0 * t
   local yval = y(x)
   if yval < 0.0 then
      yval = 0.0
   end
   return {x, yval, 0.0}
end
```

Notes:

- global variables unless stated otherwise
- can return tables

Input script – geometry definition

```
a = Vector3:new{-1.0, 0.0}
b = Vector3:new{ 0.0, 0.0}
c = Vector3:new{10.0, 1.0}
d = Vector3:new{10.0, 7.0}
e = Vector3:new{ 0.0, 7.0}
f = Vector3:new{-1.0, 7.0}
ab = Line:new{a, b}; bc = LuaFnPath:new{"xypath"} -- lower boundary in
surface
fe = Line:new{f, e}; ed = Line:new{e, d} -- upper boundary
af = Line:new{a, f}; be = Line:new{b, e}; cd = Line:new{c, d} -- vertic
-- Mesh the patches, with particular discretisation.
ny = 60
clustery = RobertsFunction:new{end0=true, end1=false, beta=1.3}
clusterx = RobertsFunction:new{end0=true, end1=false, beta=1.2}
grid0 = StructuredGrid:new{psurface=makePatch{fe, be, ab, af},
                           cfList={nil,clustery,nil,clustery},
                           niv=17, njv=ny+1}
grid1 = StructuredGrid:new{psurface=makePatch{ed, cd, bc, be},
                           cfList={clusterx,nil,clusterx,clustery},
                           niv=81, njv=ny+1}
```

Note:

- alternatively, could import grids

Input script – flow domain with boundary conditions

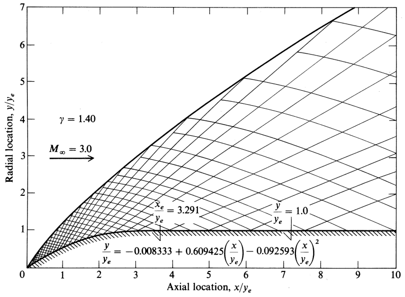
```
-- Define the flow-solution blocks.
blk0 = SBlock:new{grid=grid0, fillCondition=inflow}
blk1 = SBlock:new{grid=grid1, fillCondition=initial}
-- Set boundary conditions.
identifyBlockConnections()
blk0.bcList[west] = InFlowBC_Supersonic:new{flowCondition=inflow}
blk1.bcList[east] = OutFlowBC_Simple:new{}

config.max_time = 15.0e-3  -- seconds
config.max_step = 2500
config.dt_init = 1.0e-6
```

Notes:

- We have separated grid generation from block definition.
- fillCondition could be given as a (user-defined) function of position (x,y,z).
- Also, could provide lists of boundary conditions to the block constructors.

Result – pressure field



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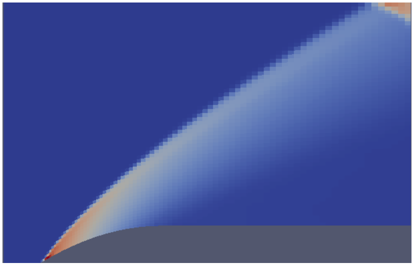
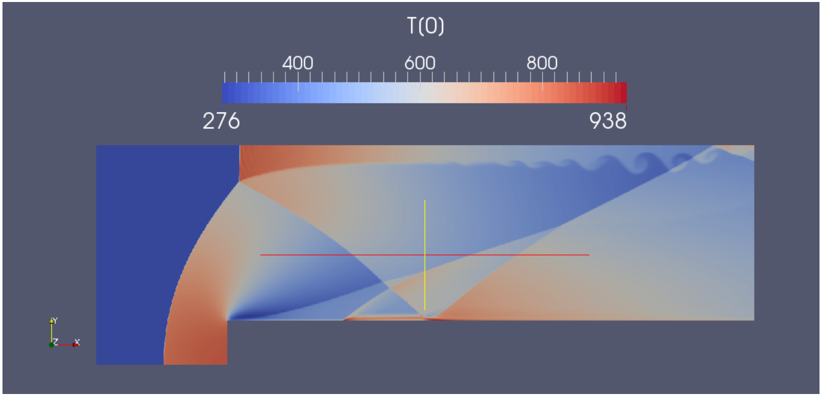


Example 2: supersonic flow over a forward-facing step



Note:

- Hurry up and show the animation.