A Sharp Interface Finite Volume Method for Variable Density Zero Mach Number Two–Phase Flow with Soluble Surfactants

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Our project objective within the SPP

Work packages

1. *Sharp interface* Finite Volume projection method
2. *Sharp interface* Poisson solver for arbitrary ratio of coefficients
3. Conservative discretization of the surface surfactant equation

plus

everything in a parallel AMR framework

Our project objective within the SPP

A Sharp Interface Finite Volume Method for Variable Density Zero Mach Number Two–Phase Flow with Soluble Surfactants (= Surface active agent)

⇒

Development of a locally second order conservative finite volume method for immiscible two-phase flow with the following features:

- sharp resolution of discontinuities
  - cut cells
  - combined conservative levelset - volume of fluid approach
- asymptotics based Poisson solver
- variable, surfactant dependent surface tension
- conservative discretization for the surface surfactant equation

Governing equations

Zero Mach-number variable density equations (Klein et al., 2001)

non-dimensional compressible Navier-Stokes equations

$+$

asymptotic expansion of primitive variables in Mach number
(e.g. $p = p^{(0)} + Ma \cdot p^{(1)} + Ma^2 \cdot p^{(2)} + ...$)

$+$

separately equating only terms of same order of magnitude in Mach number due to $\lim_{Ma \to 0}$

$\Rightarrow$

- $\nabla p^{(0)} = 0 \quad \rightarrow \quad p^{(0)} = p^{(0)}(t)$
- $\nabla p^{(1)} = 0 \quad \rightarrow \quad p^{(1)} = p^{(1)}(t)$
- leading order system ($\rho^{(0)}$, ...) contains $p^{(2)}$ in mom. eq.
- divergence constraint from energy equation
- decoupling from acoustic phenomena

Governing equations

Zero Mach-number variable density equations – leading order system

mass :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

spec :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho Y_s\,\mathrm{d}V = -\int_{\partial\Omega}\rho Y_s\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S - \int_{\partial\Omega}\boldsymbol{j}_s\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\dot{\sigma}_s\,\mathrm{d}V$$

mom :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\boldsymbol{v}\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S - \int_{\partial\Omega}p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\rho\boldsymbol{g}\,\mathrm{d}V + \int_{\partial\Omega}\mathbf{T}\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\partial\Omega\cap\partial\Sigma}\sigma\boldsymbol{t}\,\mathrm{d}l$$

energy (to be integrated):

$$(\nabla\cdot\boldsymbol{v}) = -\frac{1}{\rho c^2}\frac{\mathrm{d}p^{(0)}}{\mathrm{d}t} + \frac{1}{\rho c^2\,\Xi}\left[\nabla\cdot\boldsymbol{q} + \sum_s \boldsymbol{j}_s\cdot\nabla h_s + \sum_s \Delta h_s\dot{\sigma}_s\right]$$

Governing equations

Zero Mach-number variable density equations – leading order system

mass :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

spec :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho Y_s\,\mathrm{d}V = -\int_{\partial\Omega}\rho Y_s\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S - \int_{\partial\Omega}\boldsymbol{j}_s\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\dot{\sigma}_s\,\mathrm{d}V$$

mom :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\boldsymbol{v}\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S - \int_{\partial\Omega}p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\rho\boldsymbol{g}\,\mathrm{d}V + \int_{\partial\Omega}\mathbf{T}\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\partial\Omega\cap\partial\Sigma}\sigma\,\boldsymbol{t}\,\mathrm{d}l$$

energy (to be integrated):

$$(\nabla\cdot\boldsymbol{v}) = 0$$

Governing equations

Zero Mach-number variable density equations – hyperbolic part – advection

mass :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

spec :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho Y_s\,\mathrm{d}V = -\int_{\partial\Omega}\rho Y_s\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S - \int_{\partial\Omega}\boldsymbol{j}_s\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\dot{\sigma}_s\,\mathrm{d}V$$

mom :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\boldsymbol{v}\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S - \int_{\partial\Omega}p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\rho\boldsymbol{g}\,\mathrm{d}V$$
$$+\int_{\partial\Omega}\mathbf{T}\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\partial\Omega\cap\partial\Sigma}\sigma\boldsymbol{t}\,\mathrm{d}l$$

energy (to be integrated):

$$(\nabla\cdot\boldsymbol{v}) = 0$$

Finite Volume Projection Method

Overview

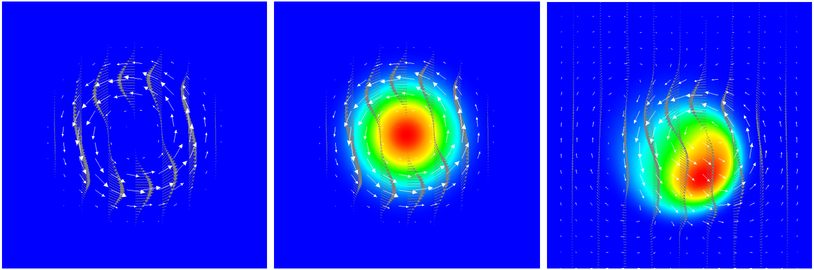
- **Predictor** (2-stage Strong Stability Preserving Runge-Kutta scheme; Gottlieb et al. 2001)
  - scalars 2nd order accurate (density, species ...)
  - old time level pressure in momentum equation
  - momentum 1st order accurate
  - no divergence constraint imposed
  - tracking of divergence error using one more transport equation
- **Corrector**
  - 1st projection (cell centered Poisson problem)
    - divergence constraint
    - correction of advective fluxes
      → scalars done after this step
  - 2nd projection (nodal Poisson problem)
    - correction of pressure term in momentum equation
      → momentum 2nd order accurate

Finite Volume Projection Method

Convergence - 2-D

Test case: Smoothed Gresho Vortex (Gresho 1990)

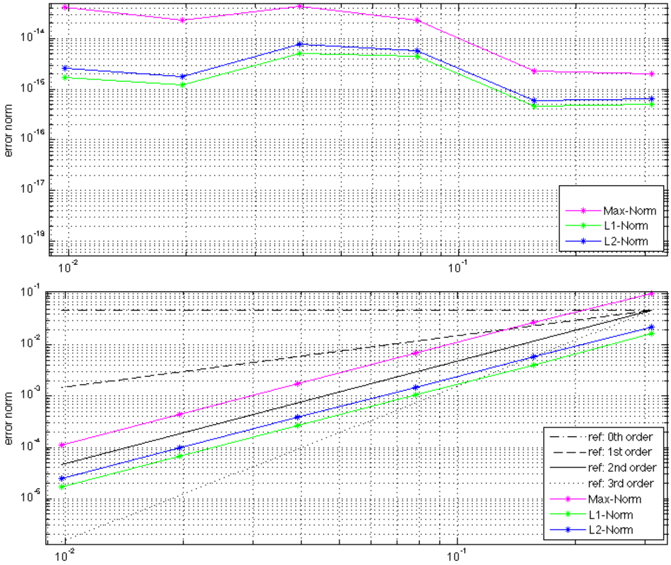
const. dens. / no grav. | no grav. | with grav.



A | B | C

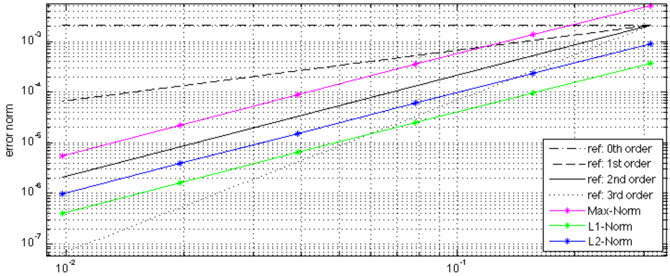
Finite Volume Projection Method

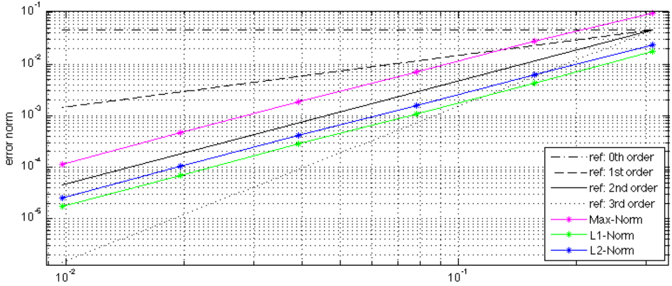
Convergence - 2-D - case A



Finite Volume Projection Method

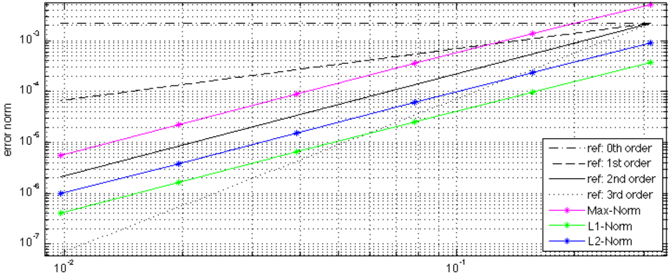
Convergence - 2-D - case B

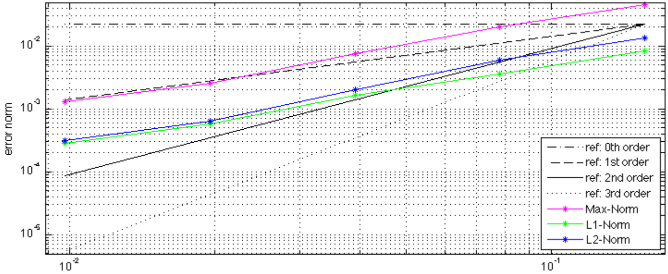




Finite Volume Projection Method

Convergence - 2-D - case C

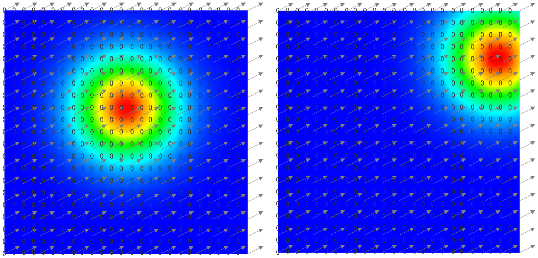




Finite Volume Projection Method

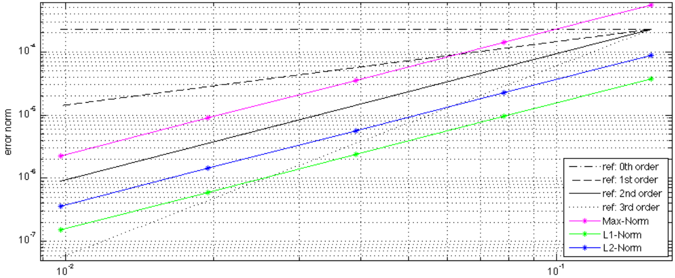
Convergence - 2-D - Advection

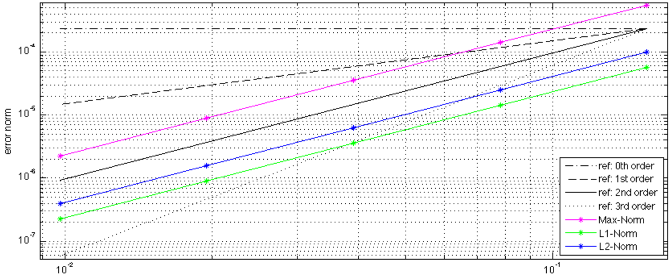
Test case: Advection Predictor only / constant pressure (0) / no gravity



Finite Volume Projection Method

Convergence - 2-D - Advection

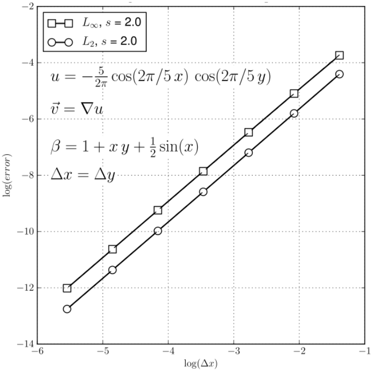




Arbitrary Ratio of Coeff. Poisson Solver

Convergence - 2-D - Node Poisson Solver

Node Poisson Solver



Finite volume formulation

$$\int_{\partial\Omega} \beta\,\nabla u \cdot \boldsymbol{n}\,\mathrm{d}S = \int_{\partial\Omega} \nabla \cdot \boldsymbol{v}\,\mathrm{d}S$$

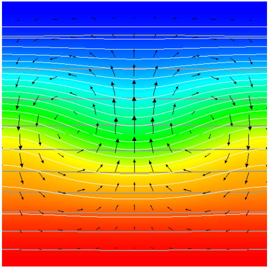
with

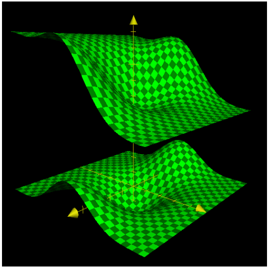
$$\nabla u \cdot \boldsymbol{n} = u_n \text{ on } \partial\Omega$$

Finite Volume Projection Method

Convergence - 2-D

Test case: Gravity Wave





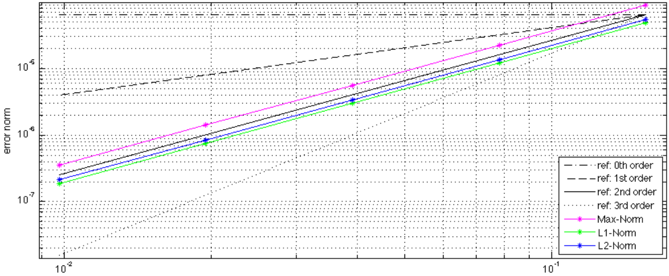
taken from

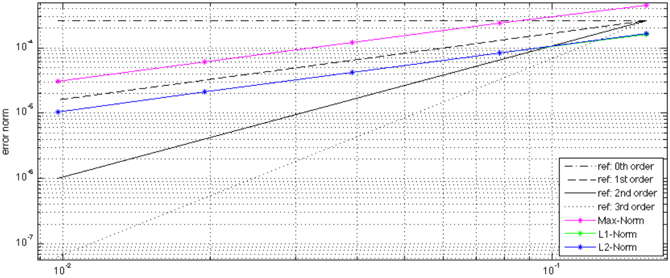
http://www.science.nasa.gov

on July 22^{nd} 2011

Finite Volume Projection Method

Convergence - 2-D - Gravity





Finite Volume Projection Method

Next Things To Do

- correct gravity term
- add boundary conditions (in-/outflow, periodic)
- add viscous terms
- bug fix 3-D
- convergence check 3-D
- complete restart capability of the code
- complete AMR capability of Poisson solvers
- add level-set and cut-cells
- implement cut-cell Poisson solver
- develope cut-cell method for solid walls
- discretization of surface tension forces
- solution of the surface surfactant equation
- surfactant dependent variable surface tension

Finite Volume Projection Method

Capabilities

- **so far**
  - conservative finite volume single phase flow solver
  - DNS, parallel (domain decomposition)
  - 2 (and 3) space dimensions
  - Cartesian grid
  - solid wall boundary conditions
  - no tubes
  - no viscous effects
- **in the end**
  - 2 and 3 space dimensions
  - two phase flow with sharp interface representation
  - arbitrarily large jumps across interface
  - Navier-Stokes equations
  - transport processes on interface for surfactant dependent surface tension
  - AMR
  - solid walls with cut-cells → tubes and complex geometries

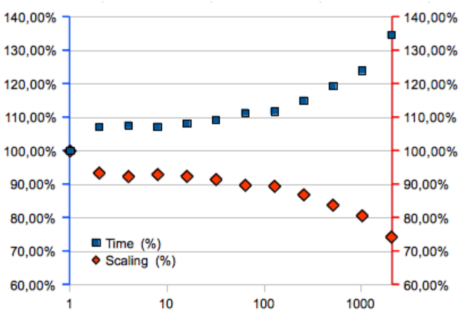
SAMRAI framework - parallel performance

Scaling test - weak scaling

weak scaling:

constant ratio between # grid cells and # processors

⇒ ideally constant computation time (proc.s keep # cells)



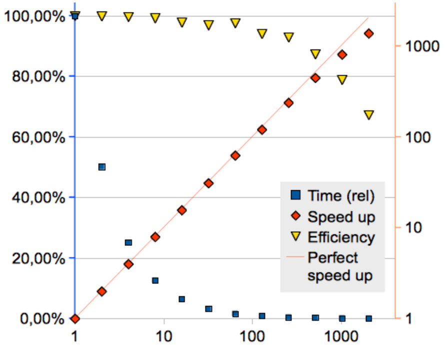
# P	# N	Time (%)	Scaling (%)
1	1	100,00%	100,00%
2	1	107,11%	93,36%
4	1	107,64%	92,91%
8	1	107,25%	93,24%
16	2	108,19%	92,43%
32	4	109,30%	91,49%
64	8	111,41%	89,76%
128	16	111,77%	89,47%
256	32	115,05%	86,92%
512	64	119,31%	83,82%
1024	128	124,01%	80,64%
2048	256	134,60%	74,29%

⇒ amount / performance of communication between proc.s

SAMRAI framework - parallel performance

Scaling test - strong scaling

strong scaling:
constant # grid cells (about 8.4 Mio. cells)
⇒ ideally constant product of computing time and # proc.s



# P	# N	Time	Speed	Effic.
1	1	100,00%	1,00	100,00%
2	1	50,11%	2,00	99,79%
4	1	25,09%	3,99	99,63%
8	1	12,60%	7,93	99,17%
16	2	6,39%	15,64	97,74%
32	4	3,23%	30,98	96,81%
64	8	1,60%	62,44	97,57%
128	16	0,83%	120,31	93,99%
256	32	0,42%	237,68	92,84%
512	64	0,22%	446,66	87,24%
1024	128	0,12%	807,01	78,81%
2048	256	0,07%	1377,68	67,27%

minimize # patches per proc. to minimize amount of inner-proc.-comm.

Finite Volume Projection Method

Limitations - as far as known so far

- maximum second order accurate
- global time step depends on smallest (regular size AMR) cell
- linear intersection in cut-cells / intersection points connected with straights
- only one intersection (interface) in a cut cell
- as long as there is not solid boundary cut-cell method implemented: geometry restrictions due to the Cartesian grid
- zero Mach (future work: switch between incompressible and compressible)
- only one set of equations for both phases
- no (input for) solid wall surface properties

Finite Volume Projection Method

Limitations - example: cut cells / AMR