Nonlinear Coupling of Thermal Explosion and Natural Convection: Numerical Simulation in Cylindrical Geometries

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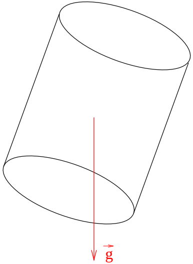
Outline

Originally: an industrial problem

Keeping potentially explosive liquid material in tanks.



Natural convection coupled with exothermal reaction.
Need to make 3-dimensional simulations,
Compute very precisely explosion limits.

Thermal explosion without free convection

Exothermic reaction: reaction rate rises with temperature, cooled boundaries.

If heat production is not balanced by heat loss at boundaries: explosion.

Frank-Kamenetskii theory

1 step reaction, Arrhenius form of the reaction rate, consumption neglected.

- Large activation energy;
- High heat of reaction.

Frank-Kamenetskii transform: [1]

scaled temperature: $\Theta = (T - T_0)E/\mathcal{R}T_0^2$,
FK: **Frank-Kamenetskii number** (efficiency of heat production)

$$\frac{\partial \Theta}{\partial t} - \Delta\Theta = \mathrm{FK}\, e^{\Theta}.$$

- $FK < 0.88$ (about 0.88) stationary stable solution.
- $FK > 0.88$ explosion.

[1] Frank-Kamenetskii, Moscow, Nauka 2nd Ed. 1967

Free convection without explosion

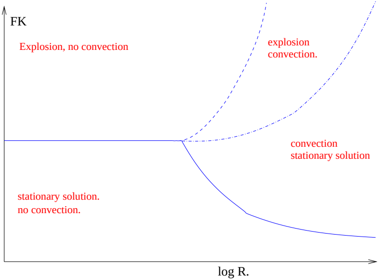
Rayleigh-Bénard configuration:
Vessel filled with a static fluid, submitted to gravity.

If heating is large enough to overcome viscous forces, convection appears.

Modeling : Boussinesq approximation.
Linear stability analysis of the static solution: convection appears as the result of a supercritical bifurcation on the **Rayleigh number** (buoyancy over viscosity).

Thermal explosion and free convection

Merzhanov-Sthessel diagram:[2]



Upper half-part of the domain: Rayleigh-Bénard problem. If $\Theta_{\max}$ is large enough: free convection.
Free convection (usually) increases heat losses through the walls: **can inhibit explosion**.

[2] Merzhanov-Sthessel. Astro. Acta, Vol.18 (1973) 191-199

Mathematical Model

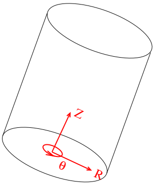
$$\rho_0 \, (\frac{\partial \vec{u}}{\partial t} + \vec{u}.\nabla\vec{u}) - \eta_0 \Delta\vec{u} + \nabla p = \beta_0 \, \vec{g} \; T \,, \qquad (1)$$

$$\nabla.\vec{u} = 0.$$

$$\rho_0 \, C_{p0} \, (\frac{\partial T}{\partial t} + \vec{u}.\nabla T\,) - \lambda_0 \, \Delta T = Q \, k \; \exp\,(-E\,/RT\,). \qquad (2)$$

+Boundary Conditions.

Spatial discretization: spectral method



- (r,z): Legendre Polynomials: $\int_{-1}^{1} P_i(x)P_j(x)dx = C_{ij}\delta_{ij}$
- θ trigonometric polynomials.

Why ?

$u \in H^k$, then $||error||_k \leq C\ N^{-k}$.

Implementation

Classical implementation: full matrices.

Idea of J. Shen:[3]
$-U'' + U = F$, on (-1,1) + homogeneous b.c.
Build a basis:
$\phi_k(x) = L_k(x) \; + \; a_k \, L_{k+1}(x) + b_k \, L_{k+2}(x)$
such that ϕ_k verifies b.c.
Then:

- stiffness matrix is diagonal
- mass matrix is penta-diagonal.

[3] Efficient Spectral-Galerkin Methods. SIAM J.Sci. Comput. Vol 18, num. 6 1583-1604, 1997

Implementation

Solution of $-\Delta\, U \;+\; \lambda\, U \;= F$ in 2d:

- 1d systems are small (method is precise!),
- Diagonalisation of matrices in one direction !

total cost for Poisson equation in 2d: $O(n\, m)$.
3d in cylinders: Fast Fourier Transform on trigonometrical polynomials:
total cost for Poisson equation in 3d: $O(n\, m\, k\;\log(k))$.

Time discretization

- highest order possible,
- low numerical cost,
- stability.

Time discretization

2nd order scheme:[4]

- $\frac{Dv^k}{Dt} = \frac{\frac{3}{2}v^k - 2\ v^{k-1} + \frac{1}{2}v^{k-2}}{dt}$ (dt is time step),
- $p^{*,k} = 2p^{k-1} - p^{k-2}$,
- $f^k = \beta_0\, \vec{g}\ T^{k+1} - \rho_0\ (u.\nabla\ u)^{*,k}$
- The scheme:

$$\begin{cases} \rho_0 \frac{Dv^{k+1}}{Dt} - \eta_0\ \Delta v^{k+1} + \nabla p^{*,k+1} = f^{k+1}, \\ (\nabla \psi^{k+1}, \nabla q) = (\frac{Dv^{k+1}}{Dt}, \nabla q)\ \forall q \in H^1(\Omega) \\ p^{k+1} = \psi^{k+1} + p^{*,k+1} - \eta_0 \nabla . v^{k+1} \end{cases}$$

solve only Poisson equations!

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[4] Guermond J-L, Shen J. A new class of truly consistent splitting schemes for incompressible flows. J. Comput. Phys. 192 (2003), no. 1

Time discretization

Heat equation:

- $g^{k+1} = Q\, k \exp^{-E/RT^{*,k+1}} - \rho_0\, C_{p0}\, (u.\nabla\, T)^{*,k+1}$,
- the scheme:

$$\rho_0\, C_{p0}\, \frac{DT^{k+1}}{Dt} - \lambda_0\, \Delta T^{k+1} = g^{k+1}$$

2nd order.

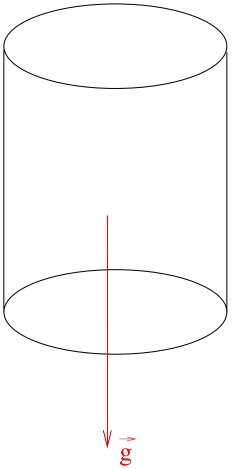
The coupled system

Time step:

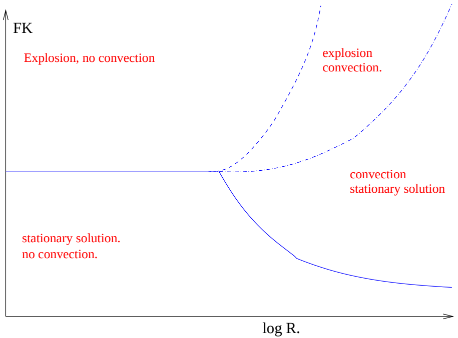
1. solve heat equation,
2. compute velocity field.

- inexpensive and precise.
- low memory cost.

first results

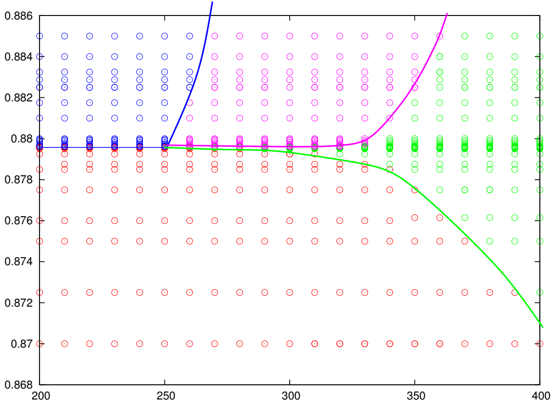


first results



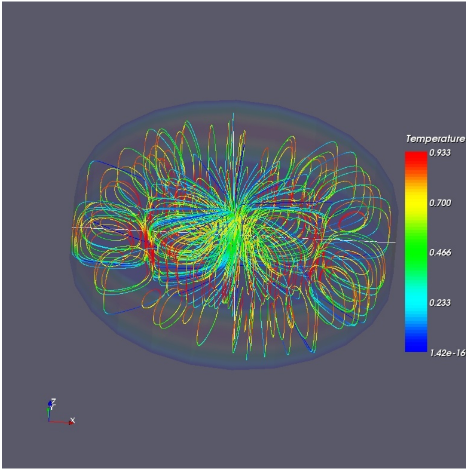
first results

The Merzhanov-Sthessel diagram in 3d:



first results

Rayleigh= 700, FK=0.87.



in progress...

- explore the complicated dynamics near the “critical” point, like in the paper of Dumont, Genieys, Massot and Volpert [5]. What happens in 3d?
- θ symetry breakdown.

[5] Interaction of Thermal Explosion and Natural Convection: Critical Conditions and New Oscillating Regimes. T. Dumont, S. Génieys, M. Massot, V. A. Volpert. SIAP, Volume 63 Issue 1 pages 351–372, 2002