Numerical Aspects in the Simulation of Thermohydraulic Transients in CICC's

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Introduction

What are thermohydraulic transients in CICC's ?



Largest time scales span

Summary

Quench studies as far back as the 70's ...

Maybe we know everything ?

- Model
- ② Discuss maths and physics
- Draw consequences for numerics
- Adaptivity
- () Conclusions

Model



Model

helium flow

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} = 0$$

$$\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho v^2)}{\partial x} + \frac{\partial p}{\partial x} = -2\rho f \frac{v|v|}{D_h}$$

$$\frac{\partial (\rho e)}{\partial t} + \frac{\partial (\rho e v)}{\partial x} + \frac{\partial (\rho v)}{\partial x} = \sum_i \frac{p_{i,He}}{A_{He}} h_i (T_i - T_{He})$$

 \mathcal{W} conduction

$$\rho_i C_i \frac{\partial T_i}{\partial t} - \frac{\partial}{\partial x} \left(k_i \frac{\partial T_i}{\partial x} \right) = \frac{\dot{q}'_i}{A_i} + \sum_{j,j \neq i} \frac{p_{j,i}}{A_i} h_{j,i} \left(T_j - T_i \right)$$

- Define time scales and characteristic lengths
- Give orders of magnitude
- Sound speed modes (pressure waves, inertia effects)



Pressure profile (pressure diffusion, friction)



Thermal Coupling (heat transfer at wetted surfaces)





Quench Propagation (front movement, free boundary)

Temperature Evolution





Quench Front Width (boundary layer)



$$k \sim 1000$$
 (W/m K)
 $v_q \sim 1-10$ (m/s)
 $\rho C \sim 1.75 \ 10^5$ (J/m³ K)
(weighted values)

characteristic length: $\lambda_q \approx \frac{k}{v_a \rho C} \sim 0.5 \text{ mm}$

Physical Characteristics - Summary

- Large disparity of time scales
- Large disparity of characteristic lengths

τ ranging from 0.5 ms to 100 s ⇒ 10⁵ λ ranging from 1 cm to 1 km ⇒ 10⁵

5 orders of magnitudes are spanned in the time/length scales

- Inspect nature of the equations
- study problems through mathematically equivalent (but simpler) models
- Hyperbolic system

$$C\frac{\partial u}{\partial t} + A\frac{\partial u}{\partial x} - G\frac{\partial^2 u}{\partial x^2} - Su = q$$

u unknowns (ρ,v,T), (p,v,T), ...

- *C* capacity matrix*G* diffusion matrix
- q source vector
- capacity matrix A convection matrix
 - *S* source matrix

A model problem

$$\frac{\partial u}{\partial t} + v \frac{\partial u}{\partial x} - \alpha \frac{\partial^2 u}{\partial x^2} = 0$$

incomprehensible defective-confusion equation (Leonard, 1979)

 $\alpha \neq 0 \Rightarrow$ parabolic equation $\alpha = 0 \Rightarrow$ hyperbolic (1st order) equation

change of *functional class* (from H^1 to H^0) depending on α !

Peclet number:



Pure Diffusion (Pe=0)



Convection-Diffusion (Pe=20)

Pure Convection (Pe=infinity)

Mathematical Characteristics - Spaces

- H^0 space of those functions that are square-integrable
- H¹ space of those functions that are *square-integrable* and whose first derivative is also *square-integrable*
- H^0 is a box of apples and pears
- H^1 is a box of apples only

 H^0 is wider than H^1

Which equations show hyperbolicity ?

helium flow



Moving Boundary

Implicit moving boundary equation $T=T_{cs}$

A model problem for pure convection

$$\frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} = \gamma H \left(T - T_{cs} \right)$$

$$\frac{\partial}{\partial t} \left[\int_{0}^{X_{q}(t)} \rho \, dx \right] = \frac{\partial X_{q}(t)}{\partial t} \rho \left(X_{q}(t) \right) + \int_{0}^{X_{q}(t)} \frac{\partial \rho}{\partial t} \, dx = 0$$

Analytic solution: moving boundary with speed $v_q = \frac{X_{q0}\gamma}{T_{cs}}$ increasing temperature with constant rate $\frac{\partial T}{\partial t} = \gamma$

- v_q is a constant
- \checkmark dependence on X_{q0} and γ (integral of source)
- the system is meta-stable (thermal runaway)



Propagation of a Model Quench

Effect of diffusion (perturbation to model problem):

$$\frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} - \alpha \frac{\partial^2 T}{\partial x^2} = \gamma H \left(T - T_{cs} \right)$$

Additional front speed





Quench propagation at <u>increasing speed</u>

Mathematical Characteristics - Summary

- strong hyperbolic character for energy balance
- sharp temperature fronts associated to both:
 hyperbolic character
 free boundary
- meta-stable system sensitive to perturbations
- pressure fronts are not expected (no shocks)
- problem is stiff (large time scale disparity)

Facts which have the *strongest* consequences:

- Hyperbolicity (significant 1st order space derivative term)
- Non-linearity, meta-stability and moving boundary
- 🖏 Stiffness

Concentrate on FD's and FE's (most flexible methods)

Remarks on other methods (few)

Hyperbolicity First trial (choice for parabolic ode's) central differences





A step back (physics of flow ?) upwind differences



Central differences in x & t \Rightarrow 2nd order of accuracy $\varepsilon = o(\Delta x^2, \Delta t^2) \frac{\partial^3 u}{\partial x^3}$ dispersion

Upwind differences in x & t \Rightarrow 1st order of accuracy $\varepsilon = o(\Delta x, \Delta t) \frac{\partial^2 u}{\partial x^2}$ diffusion

Phenomenological...Can we find a *better* explanation ?

- & FE (Galerkin) looks for a solution in H^1 (in the apple box)
- \aleph the solution is in H⁰ (apple+pears box, not an apple, a pear)

Find the apple that, in a weak sense, gives the best approximation to the pear

A bigger box (more nodes)? ⇒ A better approximation

An apple will never be a pear

- \Im FE (Petrov-Galerkin) = to FD upwind differences in x & t
- FE (Petrov-Galerkin) is optimal (1-D, steady state)
- No optimal treatment for general transient case

Moving boundary (perturbed model problem)

$$\frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} - \alpha \frac{\partial^2 T}{\partial x^2} = \gamma H (T - T_{cs})$$

1st order method:

$$\frac{\partial u}{\partial t} \approx \frac{u^{n+1} - u^n}{t^{n+1} - t^n} \qquad \qquad \frac{\partial u}{\partial x} \approx \frac{u_{i+1}^{n+1} - u_i^{n+1}}{x_{i+1} - x_i}$$

Inumerical diffusion

$$\alpha = v \left(\frac{\Delta x}{2} + \frac{v \Delta t}{2} \right)$$



desired $\alpha = 10^{-8} - 10^{-6}$ assume $\Delta x \approx v \Delta t$ (step at C=1) and v ≈ 1 m/s $\Delta \mathbf{X} \approx \Delta \mathbf{t} \approx \mathbf{10}^{-8} - \mathbf{10}^{-6} \mathbf{!}$ Length: 100 m Time span: 10 s \hat{U} Û Mesh: 100 M_{Nodes} Time steps: 10 M_{Steps} $CPUtime_{(1 CPU_{\mu}s/Node Step)} : 10^9 CPUs \implies 32 CPUy$

What is adaptivity ?

- **b** Define an error estimator (definition of ε)
- **Build a mesh designer** (Δx , Δt based on ε)
- \aleph Re-mesh until $\varepsilon < \varepsilon_{max}$

What are the problems with respect to quench simulation ?

- b No *a priori* definition of ε
- Re-meshing (may) imply iterations (non-linearity in transient)

An alternative: front tracking

Front tracking to determine desired mesh density







🖏 <u>Stiffness</u>

An example:

$$\left[\frac{\partial y_1}{\partial t} + h(y_1 - y_2)\right] = S$$
$$\frac{\partial y_1}{\partial t} + h(y_2 - y_1) = S$$

2 times scales

$$\Delta y \qquad \Rightarrow \ \tau = 1/2h \qquad < y > \qquad \Rightarrow \ \tau = S/$$

Explicit integration (Euler forward)



What are the *fast* modes (compared to τ_q)?

- pressure waves (damped by friction)
- temperature differences in the cable cross section
 $(T_{He} ≈ T_{Co})$

Implicit treatment required

non-conservative form of flow equations (p,v,T)

- Eulerian vs Lagrangian method (moving FE's)
- Packages

 solvers for systems of PDE's ⇒ scarce
 solvers for systems of ODE's ⇒ many for 2nd order
 generality ?
- Other methods ?

Numerics - Summary

Order of method (critical) first order for stability (and damping) second order for improved accuracy (a must !)

Adaptivity improves accuracy at given computational work p-h adaptivity optimal

Implicit solution

suppression of fast (useless) modes retained for generality (waves, temperature gradients)

Conclusions

Didn't we think we knew everything ?

- physical implications (compressible flow in pipes)
- mathematical implications (moving-boundary)
- numerical implications (methods' development)