SPECTRAL ELEMENT METHOD FOR THERMOCONVECTION IN A GLASS MELT

NICOLAS VANANDRUEL

Université Catholique de Louvain,
Unité de Mécanique Appliquée (CESAME), Bâtiment Euler, Av. G. Lemaître, 4-6,
B-1348, Louvain-la-Neuve, Belgium

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Accurate representation of heat and mass transfer in thermoconvective flows is of great importance in several industrial processes. In particular, this study is motivated by the need to better understand molten glass circulation in glass melting furnaces.
The geometry of furnaces is rather simple : the free surface of the molten glass is horizontal and the refractory walls are parallelepipedic. However, the flow patterns in this geometry are actually 3D as the width of the tank can be restricted at the neck while the height is modified by a step. For these reasons, the solution in the plane of symmetry can no longer be regarded as representative.
For this class of problems, the convective currents are moderate amplitude, with a typical value of Reynolds number of O(1), while the Péclet number can be of order of 300 (given the low conductivity of molten glass). The numerical difficulty is therefore associated with solving of energy equation rather then that of momentum.
While a detailed, steady-state solution is important, the time evolution of the flow structure is also of great interest. Given the intensity of the thermoconvection - the Grasshof number is ≈ 5000 - no unstationary solution should be expected. However, a sensitivity study is a variation of the solution under varying operating conditions, e.g. pull rate, thermal boundary conditions..., sheds light on the stability and the relative importance of both thermal and viscous effects.
The numerical tool developed to simulate this physical situation is an ***unstationnary spectral element*** *Boussinesq solver. Spatial discretization is realized through the division of the computational domain in a limited (<50) number of spectral elements. On each element, the unknowns are interpolated by a high-order Legendre polynomial. Depending on the value of the Prandtl number of the fluid, a greater number of degrees of freedom can be associated to the thermal problem.*
The goal of this presentation is to claim the efficiency of high order methods for the numerical simulation of thermoconvection in the glass melting tank.. Comparisons with finite-difference and finite-element solutions demonstrates a lower number of degrees of freedom necessary to obtain specified level of accuracy. A global increase in computing efficiency allows 3D simulations like time evolution of melting tank during change of glass.

NUMERICAL SIMULATION MODELS OF GLASS MELT THERMOCONVECTION

As pointed out in [4], the main problems with 3-D numerical furnace models are not only their need of computational resources - CPU and memory - but also the relative unreliability of input data (conductivity) and the limited possibilities of verification associated with difficult representation of complex solutions.

Efficient high-order methods produce accurate numerical representations within the computational environment of modern computer work station. In this environment, various graphic capacities can handle the results and allow easier interpretation of flow patterns. The problem of unreliable data can be solved by expensive "parameter studies" where successive simulations can be compared, identified with reduced scale models or even with industrial measurements. Another interesting way of using the powerful (but still approximate) numerical tool is in combination with control/identi-fication procedures. In this combined study, exchanges between unsteady numerical simulations and control/iden-tification models can be useful to gain a global understanding of the melt convection and to estimate quality-related parameters such as the temperature profile or the residence time distribution [1].

SPECTRAL METHODS

The fundamental principle of spectral methods [2] is the decomposition of the unknown fields in a linear combination of a set of basic function

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$$u_N(x) = \sum_{n=0}^{N} a_n \psi_n(x) \quad , \qquad (1)$$

where u_N is the approximation of the Nth order, the set $\{a_n\}$ is the so-called "spectrum" of this solution with respect to spectral basis ψ_n.

While, for low order methods, the basic functions are usually defined such that the $\{a_n\}$ set is actually the set of the values of the function u_N at given points (nodes); for spectral methods this simple relationship does not hold. To evaluate, from the spectrum, the values of the function at given spatial coordinates, an explicit evaluation of the fundamental decomposition is to be used. The computational cost of such an evaluation has been drastically reduced in the case of the Fourier spectral method. For this well-known particular choice of basic functions

$$\psi_n(x) = \cos \pi\, n(x-a)/L \quad , \qquad (2)$$

where $L = b - a$ is the length of the interval $[a,b]$ on which u_N is defined; the relationship between the spectrum and the value of the u_N approximation at the N equally spaced collocation points

$$x_n = a + n(b-a)/(N+1) \qquad (3)$$

has been optimized and requires only $O(N\log N)$ operations rather then $O(N^2)$ operations needed by the direct calculation. This evaluation algorithm has been called for this reason the Fast Fourier Transformation (FFT) and historically justifies the interest of spectral methods for scientific computational methods.

There is a strong dependence of the set of basic functions ψ_n on the set of collocation points where the function can be directly evaluated. While Fourier basis functions are associated with equally spaced points, Chebyshev function produce a set of points with notable refinements near the boundaries. This particularity can be advantageous when greater gradient variations (like boundary layers) are expected at the extremities of the computational domain. A third choice, the Legendre functions, present other interesting properties explained later.

Within this general framework, spectral methods are resolved with the following algorithm : *i*) the set of partial differential equations is rewritten for the spectrum of the unknown fields; *ii*) the resulting "spectrum system" is solved; and finally *iii*) the value of the u_N approximation is evaluated at the collocation points. The industrial applicability of spectral methods is severely restricted by three limitations:

- the computational domain must be "simple", i.e. topologically equivalent to a parallelepipedic box. Several domain decomposition methods have been proposed for the for the extension of spectral methods to multidomain calculations, but they suffer from difficulties arising from continuity boundary conditions at the interfaces between subdomains.
- the coefficient of the original spatial equations must be constant to allow direct transformation of the equations from the spatial to the spectral space. The conductivity and viscosity must therefore be constant on the whole computational domain.
- great numerical difficulties appear when solving the spectral set of equations. For this reason different preconditioning strategies have been investigated, leading to linear systems with better numerical conditioning.

Despite this restrictions, spectral methods has shown impressive resolution capacities for different situations such as atmospheric turbulence, crystal growth thermoconvection, and molten tin current for float glass production.

The most important feature associated with spectral methods is their convergence rate, defined as the error decrease associated with an increase in the number of degrees of freedom (d.o.f.). Low order methods typically present linear or quadratic convergence rates i.e. multiplying the number of d.o.f. by a factor of 2 divides the resulting error by 2 or 4. On the other hand, spectral methods achieve *exponential convergence rates*, i.e. the error decreases like e^{-N}, where N is the order of the approximation. Consequently, the computational effort required to attain a given level of accuracy is usually much smaller for the spectral methods, subject to the restriction that the physical situation admits the limitations of a constant-coefficient mono-domain problem.

Another useful property of spectral methods is the *a priori* error indication provided by the spectral decomposition. The last terms in the spectrum $\{a_n\}$ must be small and decreasing to ensure that the spectral approximation embodies all the meaningfull physical information.

To conclude this extremely rapid overview of spectral methods, it must be mentioned that the usefulness of this class of numerical tools has been increased by the *pseudospectral* algorithm. This algorithm avoids evaluations of the spectrum and manipulates only values of the function at the collocation points. Pseudo-spectral methods allow Legendre and Chebyschev functions to be used even through they do not have a immediate fast transform (such as the FFT in the Fourier case).

SPECTRAL ELEMENT METHOD

The spectral element method combines the exponential convergence of spectral methods with the geometrical flexibility of finite elements [5]. To achieve

this result, the variational form of the problem is solved rather then its spectral transform. If the differential system is

$$L(u) = f \tag{4}$$

then, classically, the variational (or weak form) is obtained by integration of the system with multiplication by a given weight function. The selected weight function is here the basis function ψ_n, leading to the Galerkin formulation

$$\int (L(u_N) - f)\, \psi_n = \int (L(\sum_{n=0}^{N} a_n \psi_n(x) - f)\, \psi_n = 0 \quad . \tag{5}$$

The consequences of this numerical artifacts is

- to allow the decomposition of the domain in subdomains where a spectral discretization is performed. Natural continuity of the solution through interfaces is obtained by the decomposition of the integral on each separated spectral element (through the so called "direct stiffness summation"),
- to express flux boundary condition resulting from the classical integration by parts.

Variational form is also one of the principles of the finite element methods (FEM), but while FEM generally consider a great number of small subdomains (elements) where low order interpolants approximate the unknown fields; spectral element methods (SEM) use high order spectral basis function on a moderate numbers of subdomains [6].

The function ψ_n used for this spectral elements discretization is the set of Legendre functions. Their useful characteristic is their orthogonality

$$\int_{-1}^{+1} \psi_m \psi_n = \delta_{mn} \quad , \tag{6}$$

where δ is the Kronecker symbol, leading to a diagonal mass matrix and allowing geometrical deformation of the mesh through the classical Jacobian transformation. Combined with this choice of basic function, spectral element methods select the pseudospectral algorithm.

Differences between SEM and h-type FEM lies in the interpolation order (for a furnace simulation, orders like 15 are usual) and the use of *tensorisation*. Tensorisation is the key for practical efficiency of spectral methods. Suppose we want to know the value of 3-D basis function at given location (x, y, z). Instead of naive calculation

$$\psi_{i,j,k}(x, y, z) \tag{7}$$

we use the tensor form to obtain

$$\psi_{i,j,k}(x, y, z) = \psi_i(x) * \psi_j(y) * \psi_k(z) \tag{8}$$

and reduce the cost of such estimation from $O(N^6)$ to $O(N^4)$ operations. This reduction is the main reason for the use of iterative solvers combined with spectral element methods. Those solvers, requiring limited memory, do not suffer from the "full" matrix structure of the spectral operators which couple a great number of unknowns. Logically, the resolution strategy of non-linear problems will therefore be a time dependent discretization even if the desired solution is a steady state.

GLASS THERMOCONVECTION

According to the particularities of the numerical simulation of glass thermoconvection, specific numerical techniques have been used in conjunction with spectral element methods. These techniques consider the differences both in time and space, between the temperature, velocity, and pressure fields.

From the spatial point of view, it is well known that while steep temperature gradients are encountered near the boundaries, the velocity distribution usually does not produce a boundary layer. The ratio between thermal and velocity boundary layers is measured by the Prandtl number for which a typical glass melt value is in the range of 200 to 300. For this reason, different interpolation degrees have been selected for temperature and velocity fields. For finite elements [8], quadratic temperature and linear velocity interpolations produce accurate results at low CPU cost. In this spectral element method, we select a more adaptative distribution of the number of d.o.f. In general, the temperature field requires mode d.o.f. and a typical distribution is 15 temperature for 10 velocity unknowns. However, in the width direction of the furnaces [7] where moderate values (≈ 5) are chosen, equivalent distribution is selected for temperature and velocity.

The pressure field acts, in this incompressible flow problem, as a Lagrangian multiplier to ensure vanishing velocity divergence. The value of the pressure itself is not really pertinent and moreover it does not differ much from the hydrostatic solution

$$p \sim p_0 - \rho\, g\, h \quad , \tag{9}$$

where h is the depth and p_0 the atmospheric pressure. Therefore, several methods can be used [3] to ensure incompressibility without explicitly calculating the superfluous pressure fields.

Similar differences between velocity, temperature, and pressure are realized for the time discretization. As quantified in [8], the Prandtl number also is a measure of the ratio between velocity and temperature time constants τ_{vel} and τ_{temp}. Selecting the following approximations, which can be verified by numerical experiments,

$$\tau_{vel} \sim L^2/\upsilon \text{ and } \tau_{temp} \sim L^2/\kappa \ , \qquad (10)$$

where υ is the kinematic viscosity, κ the thermal diffusivity and L typical length, the ratio τ_{temp}/τ_{vel} reduces simply to the Prandtl number υ/κ. The velocity time step is therefore smaller than that for the temperature, a good compromise being about 10 velocity time steps for each temperature. The pressure problem is only resolved when the velocity divergence becomes greater than a given tolerance value.

With all these numerical techniques, a required accuracy level can be reached within acceptable CPU costs. Consequently, different unsteady simulations can be realized, including changes of the operating conditions and mixing. On the other hand, a highly accurate solution - obtained with voluntary "excess" of d.o.f. - is a powerful tool for numerical quality dependent studies like tracking or residence time evaluations [1]. The global approach of the spectral element method, rapidly ensuring grid independence, appears therefore as a good candidate for glass thermoconvection simulations.

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POUŽITÍ METODY SPEKTRÁLNÍCH PRVKŮ PŘI ŘEŠENÍ KONVEKCE TEPLA VE SKLOVINĚ

NICOLAS VANANDRUEL

Unité de Mécanique Appliqueé (CESAME), Université Catholique de Louvain, Bâtiment Euler, Av. G. Lemaître, 4-6, B-1348 Louvain-la-Neuve, Belgium

Přesné vystižení přenosu tepla a hmoty při termokonvekčním proudění je velmi žádoucí u mnoha druhů průmyslových procesů. Tento příspěvek je zaměřen zejména na lepší pochopení proudění skloviny ve sklářských pecích.

Geometrie těchto pecí je dosti jednoduchá : volná hladina skloviny je horizontální, a stěny ze žáruvzdorných materiálů mají v podstatě tvar hranolu. Skutečné profily proudění jsou však ve skutečnosti trojrozměrné, neboť šířka vany bývá zúžená v místě krku, a hloubka skloviny zároveň snížená stupněm. Z těchto důvodů nelze považovat za vyhovující řešení založené na plošné souměrnosti.

U tohoto okruhu problémů vykazuje konvekční prodění menší amplitudy, s typickou hodnotou Reynoldsova čísla O (1), zatímco Pécletovo číslo může mít řádově hodnotu 300 (vzhledem k nízké tepelné vodivosti skloviny). Obtíže s modelováním proto spíše souvisejí s rovnicí přenosu energie než s rovnicí přenosu hybnosti.

I když je řešení v ustáleném stavu důležité, časový rozvoj průběhu proudění je rovněž významný. Při dané intenzitě přenosu tepla konvekcí (Grasshofovo číslo má hodnotu cca. 5000) nelze očekávat nestacionární řešení. Studie citlivosti, se kterou kolísají výsledky za různých provozních podmínek, například při různém průtoku, nebo při různých teplotních okrajových podmínkách, však poskytuje informace o stabilitě výpočtu a relativní důležitosti jak tepelných, tak viskozitních faktorů.

Výpočetním nástrojem vyvinutým pro modelování této fyzikální situace je metoda Boussinesq solver, poskytující přímé řešení a využívající nestacionární spektrální prvky. Prostorová diskretizace se realizuje rozdělením výpočtové domény do omezeného počtu (<50) spektrálních prvků. Pro každý prvek se neznámé interpolují Legendrovým polynomem vysokého řádu. V závislosti na hodnotě Prandtlova čísla příslušné tekutiny lze přenosu tepla přiřazovat vyšší počet stupňů volnosti.

Cílem tohoto příspěvku je prokázat efektivnost metod vyššího řádu pro matematické modelování teplotní konvekce ve sklářské vanové peci. Porovnání s výsledky řešení pomocí konečných rozdílů a konečných prvků ukazuje, že pro dosažení požadované přesnosti lze použít menší počet stupňů volnosti. Celkové zvyšování výkonů počítačů umožňuje trojrozměrné modelování v neustáleném stavu, jako například modelování časového průběhu změny druhu skloviny ve vanové peci.