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Direct Numerical Simulation of Boiling Multiphase Flows: State-of-the-Art, Modeling, Algorithmic, and Computer Needs

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Direct Numerical Simulation of Boiling Multiphase Flows: State-of-the-Art, Modeling, Algorithmic and Computer Needs

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ABSTRACT

The state-of-the-art for Direct Numerical Simulation (DNS) of boiling multiphase flows is reviewed, focussing on potential of available computational techniques, the level of current success for their applications to model several basic flow regimes (film, pool-nucleate and wall-nucleate boiling – FB, PNB and WNB, respectively). Then, we discuss multiphysics and multiscale nature of practical boiling flows in LWR reactors, requiring high-fidelity treatment of interfacial dynamics, phase-change, hydrodynamics, compressibility, heat transfer, and non-equilibrium thermodynamics and chemistry of liquid/vapor and fluid/solid-wall interfaces. Finally, we outline the framework for the Fervent code, being developed at INL for DNS of reactor-relevant boiling multiphase flows, with the purpose of gaining insight into the physics of multiphase flow regimes, and generating a basis for effective-field modeling in terms of its formulation and closure laws.

Key Words: Boiling multiphase flows, Direct Numerical Simulation, Interface tracking, Two-fluid model.

1. MOTIVATION

Modeling of boiling multiphase flows is at the core of light water reactor safety. A variety of effective-field-based numerical codes (such as RELAP-5 [37]) have been developed with variable levels of success since the late 1970s. The main purpose of the integrated system analysis is to simulate postulated nuclear reactor accidents. On the wave of the current nuclear energy renaissance, a new set of requirements for analysis tools has emerged, emphasizing ***predictive capability***, as the future advanced nuclear energy systems (Gen-III+, Gen-IV reactors; GNEP facilities) must be designed not only with superb safety features, but also to be competitive with conventional carbon-fossil fuel technologies, necessitating optimization/increase in reactor power load and high-temperature cycles. As the design of new reactors is expected to rely heavily on numerical simulations, the "bar" for accuracy, reliability and low/quantifiable-uncertainty-margin of the future system analysis codes is set high. This requires a new philosophy of how these tools should be designed, accounting for remarkable development of numerical methods for complex PDE systems in the last 20 years, and appreciating the need for tight numerical coupling of diverse physical processes in complex engineering systems – that is, reflecting their ***Multi-Scale*** and ***Multi-Physics*** nature.

We want to describe two-phase flows in core fuel assembly, in both steady, normal operation and in transient/accident scenarios. We visualize the path towards these goals as a three-tier combination of numerical tools:

Tier I. ***Effective-field-based system analysis codes.*** These are the next generation of RELAP-like system simulation codes, incorporating the state-of-the-art numerics and physics/theory of two-fluid models.

The former includes ***a)*** *discretization of equations in a fully conservative form* (enabling mass, momentum and energy conservation regardless of chosen level for non-linear solver tolerance); ***b)*** *high-order* (at least 2^{nd}) *discretization in both time and space*; ***c)*** *fully implicit treatment*, yielding tight coupling with other physics (e.g., neutron kinetics, radiation heat transfer, structural mechanics, etc.) and accuracy at large time steps (implying efficiency and robustness in multiple-time-scale transients). The key in this effort is using the *Jacobian-Free Newton Krylov (JFNK) framework* [21] combined with development of appropriate preconditioning. All the above depend upon recent advances in two-fluid model theory, implying ***d)*** *the system of governing equations is well-posed* [7, 24, 39]. For efficiency purposes, the tools of this group involve relatively coarse nodalization and mostly/effectively 1D discretizations; therefore the closure laws should be implemented in the spirit of "flow regime maps" (for "stratified", "bubbly", "slug", "annular-mist", "inverted annular", "inverted slug", "mist", etc. regimes); as it has been done in the old-generation RELAP-family codes [37]. The important difference is that we ***e)*** *need to incorporate time and length scales into the constitutive physics* so as *to account for transient and developing regimes* as a way to reduce uncertainties in system-design and safety-margin analysis.

Tier II. ***Effective-field-based two-phase flow analysis codes.*** While these codes utilize similar numerics as the "Tier-I"-codes, they are intended to be run in *multi-dimensions with high-resolution*, with the purpose of providing details of constitutive physics for flow regime maps of the system analysis codes of Tier I. Spatio-temporal resolution should be fine enough, so the subgrid closure physics is narrowed down to a few dispersed or stratified flow regimes, which are provided by DNS codes.

Tier III. ***DNS codes for boiling two-phase flows.*** These are the continuum-mechanics, first-principle based codes*, developed accounting for all important physics of boiling flows in nuclear reactors, with the purpose of ***a)*** *gaining insight into the physics of "basic" dispersed/stratified flow regimes* (e.g., pool nucleate boiling; mist flows; wall nucleate boiling; wall droplet deposition/evaporation; film boiling/reflooding/dryout, etc.); and ultimately ***b)*** *providing a detailed database for development of empirical correlations and constitutive physics with time and length scales for the effective-field-based codes* discussed in Tiers I and II.

The purpose of this paper is to summarize recent developments in Direct Numerical Simulation (DNS) of boiling two-phase flows, and to outline the requirements and projected framework (including modeling, algorithmic and hardware needs) required for successful simulations of practical boiling flows in nuclear reactors, accounting for recent and future (projected) progress in computer science, numerical methods for complex PDE systems and understanding/diagnostics of two-phase flows.

2. STATE-OF-THE-ART

DNS of boiling flows was pioneered by Samuel Welch in 1995 [49], who developed a two-dimensional, moving-mesh finite volume method for a single, weakly-deformable bubble. Since then, the major research was concentrated in two groups: UCLA, lead by Vijay Dhir [8, 42–45]; and UoM/WPI, lead by Gretar Tryggvason [9–12, 18, 40]. Both groups base their codes on the projection methods for incompressible flows (in both liquid and vapor), extended to model boiling two-phase flows through modifications of Peskin's immersed boundary method (IBM) [35] – i.e., the liquid-vapor interface is smeared in a corridor of a few computational nodes, providing a smooth transition of fluid properties and body force for

*It is understood that some modeling is implied – such as nanophysics of thin films in wall nucleate boiling, density of nucleation sites, thermodynamics and chemistry of interface and solid walls, wall surface roughness, turbulence modeling, etc.

interfacial tension ("Diffuse Interface Method", DIM). The major difference between these two groups is how the interface is tracked – Dhir bases his code on the Level Set (LS) method [34], while Tryggvason uses his Front-Tracking (FT) approach [52]. The other DIM-based DNS studies of boiling flows are due to Welch and Wilson [50] (incompressible-flow projection method, volume-of-fluid VOF for interface tracking); Tomar et al. [48] and Mihalef et al. [27] (both with incompressible-flow projection method and hybrid of LS and VOF methods (CLSVOF) for interface tracking). To our knowledge, only two papers developed Sharp-Interface Method (SIM) for boiling two-phase flows – Ye at al. [56] combined their B-spline-based FT method with an innovative cut-cell, sharp-interface, finite-volume method; and, more recently, Gibou et al. [14] extended LS, Ghost-Fluid, finite-difference, projection method to boiling flows. There are a few other studies applying "exotic" CFD methods – such as Lattice-Boltzmann (LBGK) [53, 54], Moving-Particle Semi-implicit Gridless (MPS-MAFL) [57] and Cellular Automata SIMPLER (CAS) [55] methods.

Most of the above studies focussed on simulation of horizontal, low-temperature, near-critical ***film boiling (FB)*** [10–12, 18, 40, 42, 43, 48, 50], reproducing the well-known experimental correlations for cryogenic fluids by Klimenko [20] and Berenson [2]. Since the physics of horizontal film boiling is dominated by the Rayleigh-Taylor instability [2], all of the above incompressible methods, including some with rather severe assumptions (like neglecting heat transfer in liquid phase by Tomar et al. [48]) and smearing the interface by DIM[†‡]), performed notably well.

A few studies successfully demonstrated capabilities to simulate single- and multi-bubble dynamics in ***pool nucleate boiling (PNB)*** [27, 49, 56, 57], with mild phase change. Esmaeeli and Tryggvason [9] performed computations of violent boiling in near-critical, cryogenic, superheated fluids under zero-gravity conditions. Even with the questionable assumption of incompressible flow for explosive phenomena, they were able to reproduce structures similar to those experimentally observed by Frost [13].

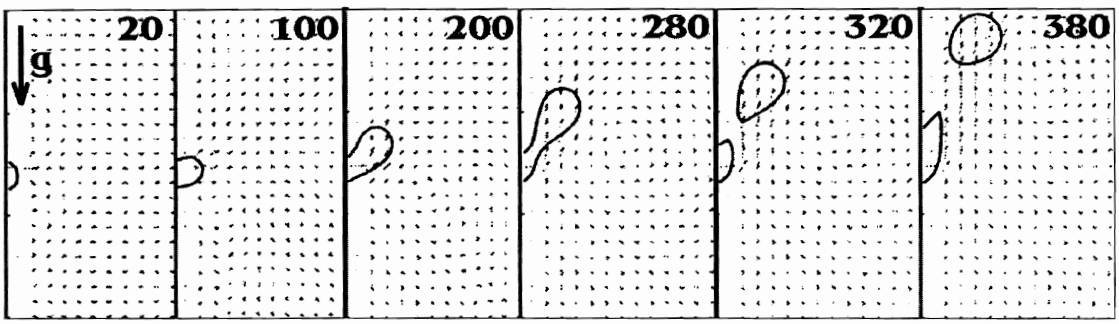

Figure 1. Illustration of bubble growth and detachment on a vertical surface. Lattice-Boltzmann simulation [53].

Simulations of ***wall nucleate boiling (WNB)*** were done by Dhir et al. in [8, 44, 45]. Since WNB is dominated by solid-wall, thin-film nanophysics[§], Dhir et al. coupled their two-dimensional DNS code with a nanofilm, lubrication-theory model. This model is applied at the base of the nucleating bubble [44] and provides the vapor mass source near the heated wall. Focusing on the dominate physics of the thin-film

[†]No significant improvement of SIM over DIM was identified by Gibou et al. [14].

[‡]As demonstrated in [33], the DIM methods perform well in Rayleigh-Taylor flows.

[§]Recent study by Theofanous et al. [46, 47] provides compelling evidences of scale separation for nanoscopically smooth surfaces, indicating unimportance of macroscale hydrodynamics for onset of CHF.

phase-change, they were able to reproduce structures of single and multi-bubble growth, departure and merger, similar to those in their experimental observations; and this is in spite of physical limitations due to the modeling assumptions of incompressibility, no conduction in the vapor phase and simplified (compared to others) modeling of interface phase change in their LS method. It is instructive to note that similarly realistic bubble dynamics were reproduced by Yang et al. [53, 55], shown in Figure 1, which involved even more severe assumptions pertinent to intrinsic limitations of the LBGK approach used. The key in all these studies was to supply appropriate wall boundary conditions for the continuity equation, rendering realistic-looking transients of macro-bubble hydrodynamics. However, without high resolution in space and time, high-fidelity physical models and tight coupling of relevant physics, it is difficult to achieve reliable predictive capabilities for heat transfer in WNB.

3. NEEDS AND PROJECTED FRAMEWORK

As discussed previously, most earlier efforts in developing numerics for DNS of boiling flows adopt variations of Chorin's projection method [6] to multiphase flows by combining them with interface tracking techniques (FT, LS, VOF or CLSVOF) and Peskin's Immersed Boundary Method (IBM). The consequences of the numerical method limitations are the set of physical model assumptions, e.g.: incompressibility, Boussinesq approximation for buoyancy, low-density ratio between phases[¶], neglection of heat conduction in one of the phases, no radiation heat transfer, low-fidelity for shear-instabilities, laminar flows, etc. Some of these physics assumptions are dictated by lack of robustness of their solution algorithm. Most of these assumptions are justifiable for their intended applications; however, they may not be adequate for nuclear reactor simulations. For example, radiation is very important heat transfer mechanism in film boiling, reflooding and dryout; high-fidelity in prediction of shear instabilities and modeling of turbulence is very important for many flow regimes during LOCA, PTS and Reactivity Accidents; compressibility must be accounted for in flow regimes of severe accidents; and so on.

As one can see from Figure 2, boiling two-phase flows are actually rather complex multiscale multiphysics problems, requiring a panoply of numerical techniques for different physics coupled together for a particular set of flow parameters and regime maps.

Our strategy in this respect is to capitalize on recent significant progress in the ***Jacobian-Free Newton Krylov method*** [21], enabling tight coupling of multiphysics and robust simulation of problems with multiple time scales. We base our temporal discretization on implicit Runge-Kutta schemes [5], which are L-stable and up to 5^{th}-order-accurate (Figure 8d). High-fidelity spatial resolution is achieved by combining Structured Adaptive Mesh Refinement (SAMR) [3, 31, 32] (Figures 3 and 4) with high-order finite-volume spatial discretization schemes (Figure 8c).

It is important to note that ***high-accuracy*** must be enforced not only in the bulk fluid, but also ***near the interface***, enabling prediction of interfacial instabilities and fidelity in simulation of boiling/condensation, breakup, coalescence, bubble detachment/merger, drop impingement, etc. For this, we will capitalize on significant progress in *Sharp Interface Methods (SIM)*, recently demonstrated to not only accurately simulate phase change in boiling flows [14, 56], but also to predict Rayleigh-Taylor and viscous Kelvin-Helmholtz instabilities [33], including the ability to self-select (for dominant growth) the naturally-preferred wavelength(s) (Figure 5) and to accurately capture growth factors and neutral stability

[¶]Sharp-Interface methods like [56] and [14] combined with Conjugate-Gradient-based linear algebra solvers permit robust solutions with realistic density ratios.

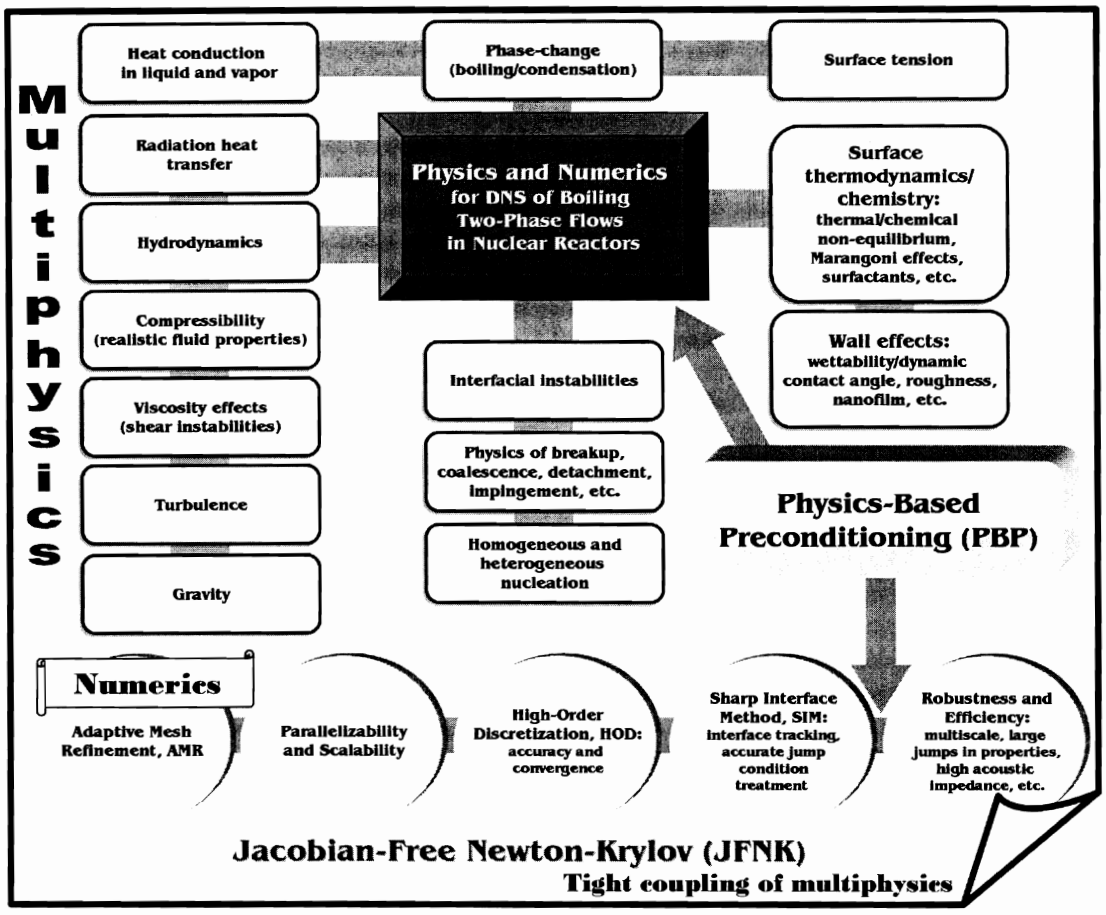

Figure 2. Outline of the projected framework for DNS of boiling two-phase flows in nuclear reactors (Fervent code).

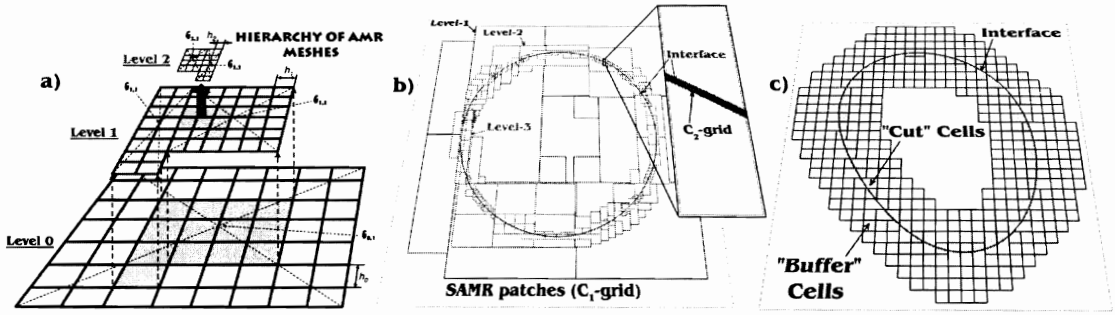

Figure 3. Illustration of Adaptive Cartesian Cut-Cell Mesh Refinement (AC^3MR) [33].

maps for Yih- interfacial instability (Figure 6). The key is in the combination of SAMR with cut-cell technology (AC^3MR, Figure 3) and 'sided, least-squares, jump-conditions-accounting' interpolation at the

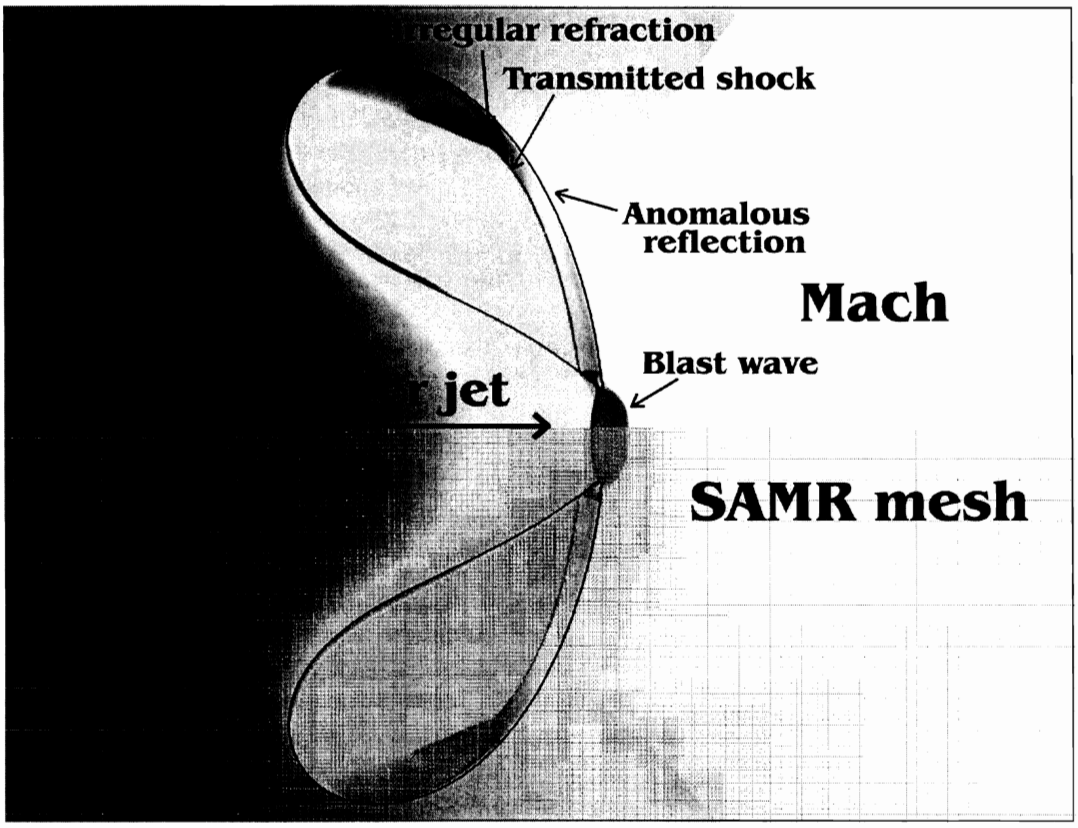

Figure 4. Simulation of shock-induced bubble collapse, using the level-set-, Characteristics-Based Matching and Structured Adaptive Mesh Refinement [31, 32].

interfacial vertices of cut cells [33], allowing for up to the 3rd-order accurate treatment of interfacial jump conditions.

Basing our linear algebra solution strategy on ***Krylov subspace iteration methods*** (like GMRES) [38] offers us significant flexibility in attacking complex multiphysics problems (Figure 2) – in particular, linear algebra is not constrained by symmetric, positive-definite (SPD) matrices[‖] (best solved by multigrid and/or conjugate-gradient methods); but rather, they allows us to address a wide spectrum of practical applications, focussing on non-linear coupling of dominant physics, including combinations of compressible hydrodynamics with phase change [36], radiation heat transfer (Figure 7), non-equilibrium surface thermodynamics/chemistry and accounting for wettability/dynamic contact angle, nanofilm-physics (by lubrication theory), turbulence modeling, etc.

The key to efficiency of the Krylov methods is the development of ***efficient physics-based preconditioners (PBP)***. In PBP, one uses traditional numerical methods developed for DNS of boiling multiphase flows as a preconditioner. The purpose of preconditioning is to cluster/collapse singular-values/eigenvalues of the Jacobian matrix [15, 38], thereby better conditioning it and helping GMRES to converge in only a few

[‖]Fedkiw's GFM [19] is one of a few interesting methods allowing to solve sufficiently complex (sharp-interface) problems preserving SPD properties of the underlying linear algebra.

Krylov iterations. There are plenty of examples of successful application of the PBP-enforced JFNK for complex physical problems [22, 28, 29, 36]. Here, we illustrate it using an Implicit Continuous-fluid Eulerian (ICE) method for all-speed flows [4, 16, 26].

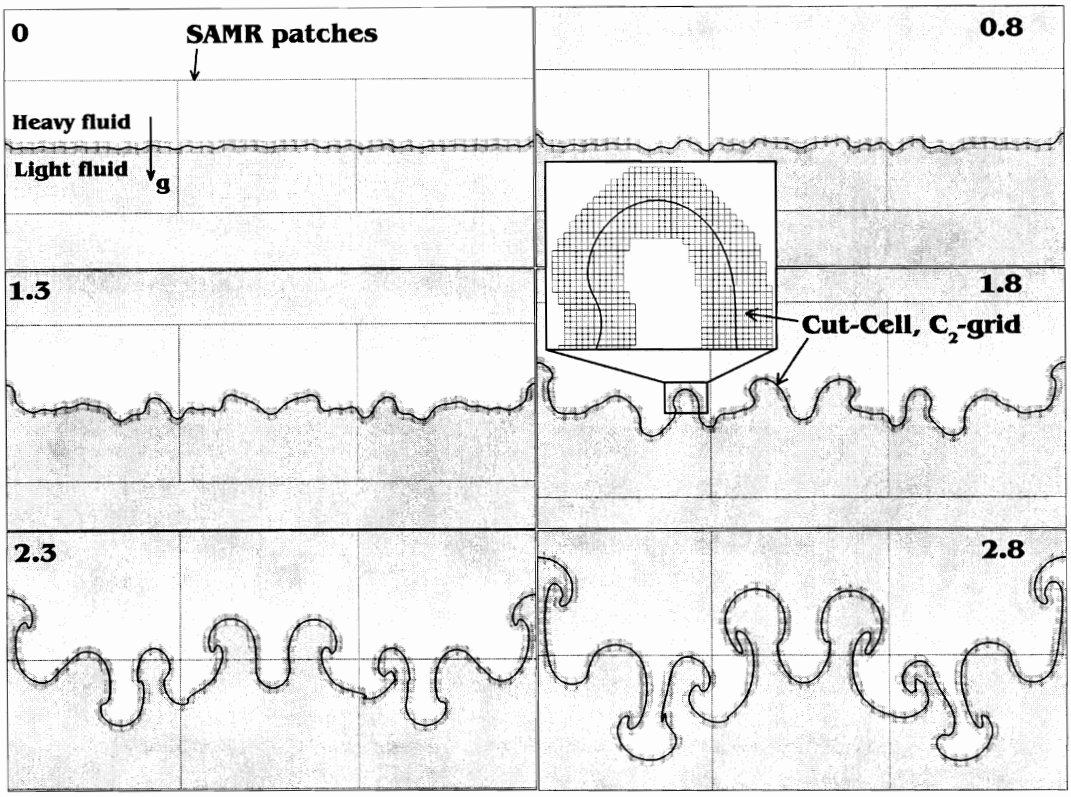

Figure 5. Numerical prediction of multi-mode Rayleigh-Taylor instability in the nearly-incompressible regime. Simulation with the level-set-based, adaptive Cartesian Cut-Cell Mesh Refinement (aC^{3}MR), Sharp Interface Method (SIM) [33]. Dynamics of interfacial shape and aC^{3}MR grid. At=1/3 (Atwood number), R=10^3 (Reynolds number), m=0.5 (viscosity ratio), r=0.5 (density ratio), no surface tension. Effective grid resolution by 2-level SAMR with refinement ratio 4 is 512 nodes/(domain width). According to linear stability theory [33], the wavenumber of the most "dangerous" wave is 5.767, which is consistent with observed here dominant wavenumber 5-6.

We use PBP-JFNK for a ***"Traveling Wave" problem*** (Figure 8a,b), which is "manufactured" [23] for compressible fluid dynamics as:

$$\begin{aligned} \rho(\mathbf{x},t) &= \rho_{\min} + (\rho_{\max} - \rho_{\min}) \operatorname{sech}\left(\tfrac{x-\omega t}{\delta}\right) \\ E(\mathbf{x},t) &= \tfrac{1}{2}\left(1 + \tfrac{2}{\gamma(\gamma-1)M^2}\right) U_0^2 \left[\rho_{\min} + (\rho_{\max} - \rho_{\min}) \operatorname{sech}\left(\tfrac{x-\omega t}{\delta}\right)\right] \\ m(\mathbf{x},t) &= U_0 \left[\rho_{\min} + (\rho_{\max} - \rho_{\min}) \operatorname{sech}\left(\tfrac{x-\omega t}{\delta}\right)\right] \end{aligned} \tag{1}$$

where (ρ, E, m) are mass, total energy and momentum densities, respectively. U_0 and M are material velocity and Mach number, both constant in space, corresponding to three constant eigenvalues of the PDE system. The pressure/density wave of thickness δ travels to the right with constant speed ω, Figure 8a,b.

Gas dynamics equations are discretized using WENO_5 scheme [17] combined with $\text{AUSM}^{+,\text{up}}$ approximate Riemann solver [25]. The Jacobian matrix $\mathbb{J}$ is non-symmetric, which excludes conjugate-gradient methods. The eigenvalues for the 2^{nd}-order Crank-Nicholson time discretization are shown in Figure 8e (black stars). It appears that eigenvalues corresponding to material velocity are concentrated on the real axis, while those due to acoustic/pressure waves are complex, forming a distorted elliptic ring. The ICE algorithm is an operator-split method designed to resolve momentum advection explicitly, and pressure waves implicitly [4, 16, 26]. Applying ICE as PBP allows one to cluster all eigenvalues of the preconditioned Jacobian matrix $\mathbb{J} \times \mathbb{P}^{-1}$ on the real axis (red circles in Figure 8e), resulting in nearly one order of magnitude faster convergence of GMRES (shown in Figure 8f for M=0.1).

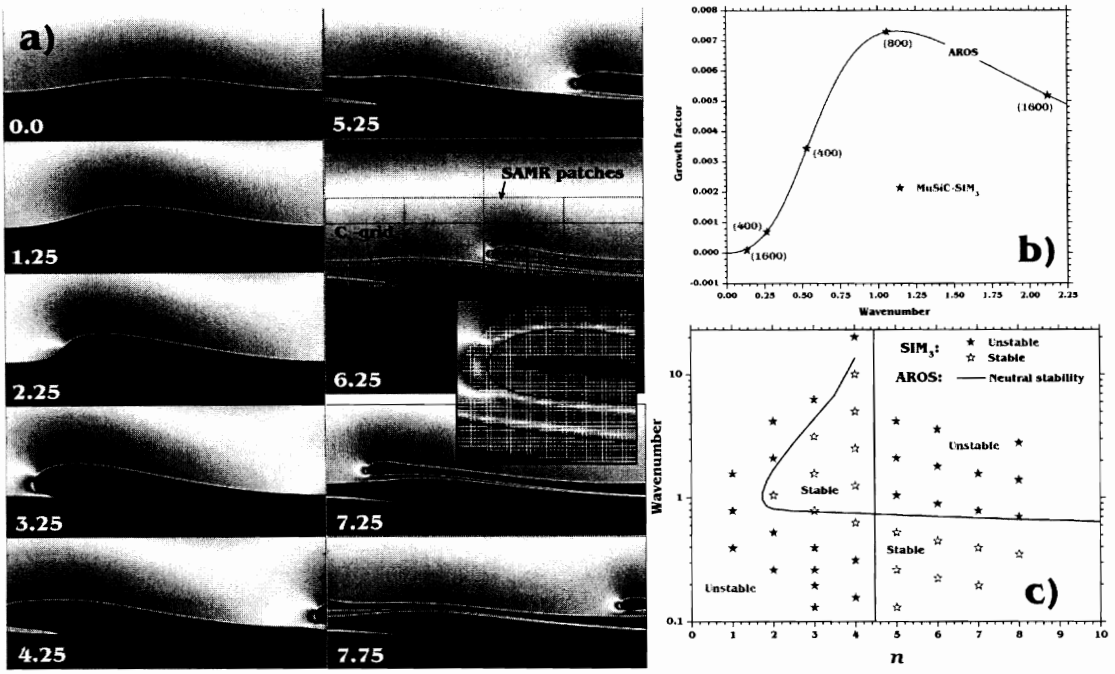

Figure 6. Numerical prediction of the viscous Kelvin-Helmholtz instability in the nearly incompressible regime. Simulation with the level-set-based, adaptive Cartesian-Cut-Cell Mesh Refinement (aC^{3}MR), Sharp Interface Method (SIM) [33]. a) Dynamics of the interface and vorticity field. Structure of the aC^{3}MR grid is exemplified for t=6.25. Effective grid resolution by 4-level SAMR with refinement ratio 2 is 400 nodes/wavelength. R=10 (Reynolds number), m=20 (viscosity ratio), r=1 (density ratio), n=1 (fluid depth ratio), $\alpha = \pi$ (wavenumber), no surface tension. b) A comparison of linear stability theory (AROS code) and SIM$_3$-based DNS. R=0.009, m=0.203, r=1, S=0, n=4.875, $\varepsilon^*_{\text{KH}}(0) = 1.175 \cdot 10^{-3}$. SIM's effective grid resolutions (# of nodes per λ) are shown in parentheses. c) Neutral stability map for the Yih-mode. R=10, m=20, r=1, S=0. Comparison of SIM with linear theory (AROS code).

Parallelizability and scalability of the solution algorithm is a major concern due to challenging super-scale-simulation requirements for DNS of boiling multiphase flows. In this regard, we capitalize on availability of advanced parallel high-performance packages for numerical solution of PDE systems

(ANL's PETSc [1]) and parallel Adaptive Mesh Refinement frameworks (like LLNL's SAMRAI [51]). While super-scale simulations of the *developing and transient complex flow regimes and their transitions* appear to be challenging at the moment, the recent tendencies in hardware and numerical algorithm improvements indicate feasibility of the "Petascale Computing" in a few years** which would make these computations practical.

4. CONCLUSIONS

Recent significant progress in computer science and numerical methods for complex PDE systems indicates feasibility of large-scale first-principle-based simulations of extremely challenging multiscale, multiphysics problems. Two-phase boiling flow is one of these, and the ability to ***predict*** developing and transient flow regimes is seen to have a significant impact on both *understanding the physics* of multiphase flows and *increasing fidelity of system analysis codes* for light water reactor safety.

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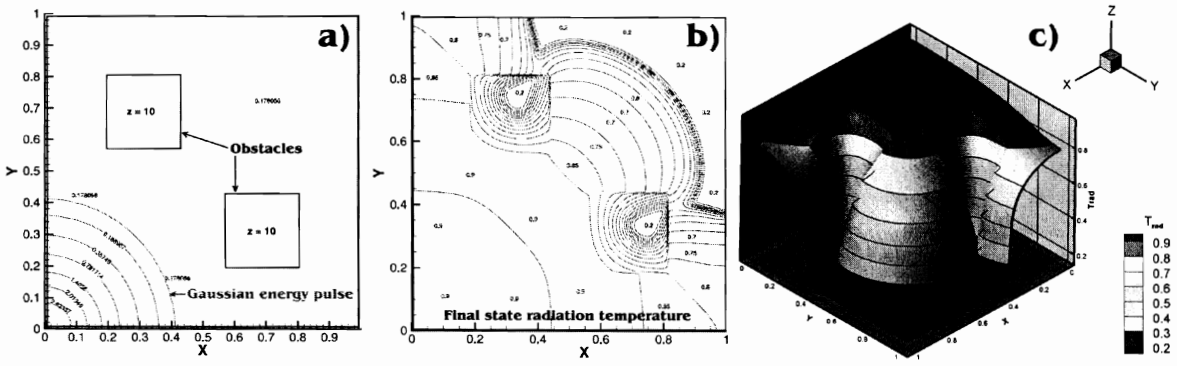

Figure 7. Illustration of the nonequilibrium radiation-diffusion problem solved with JFNK [30]. The initial Gaussian energy pulse in radiation temperature is shown in (a). The energy pulse has spread until it has engulfed the two obstacles and achieved the state shown in (b,c).

** *"Together with Stephen Jardin of the Princeton Plasma Physics Laboratory, David Keyes (a computational mathematician at Columbia University and acting director of the Institute for Scientific Computing Research (ISCR) at Lawrence Livermore National Laboratory) developed a breakdown that explains where as many as 12 orders of magnitude of speedup will come from over the next decade: 1.5 from increased parallelism, 1.5 from greater processor speed and efficiency, four from adaptive gridding, one from higher-order elements, one from field-line following coordinates, and three from implicit algorithms."* [41].

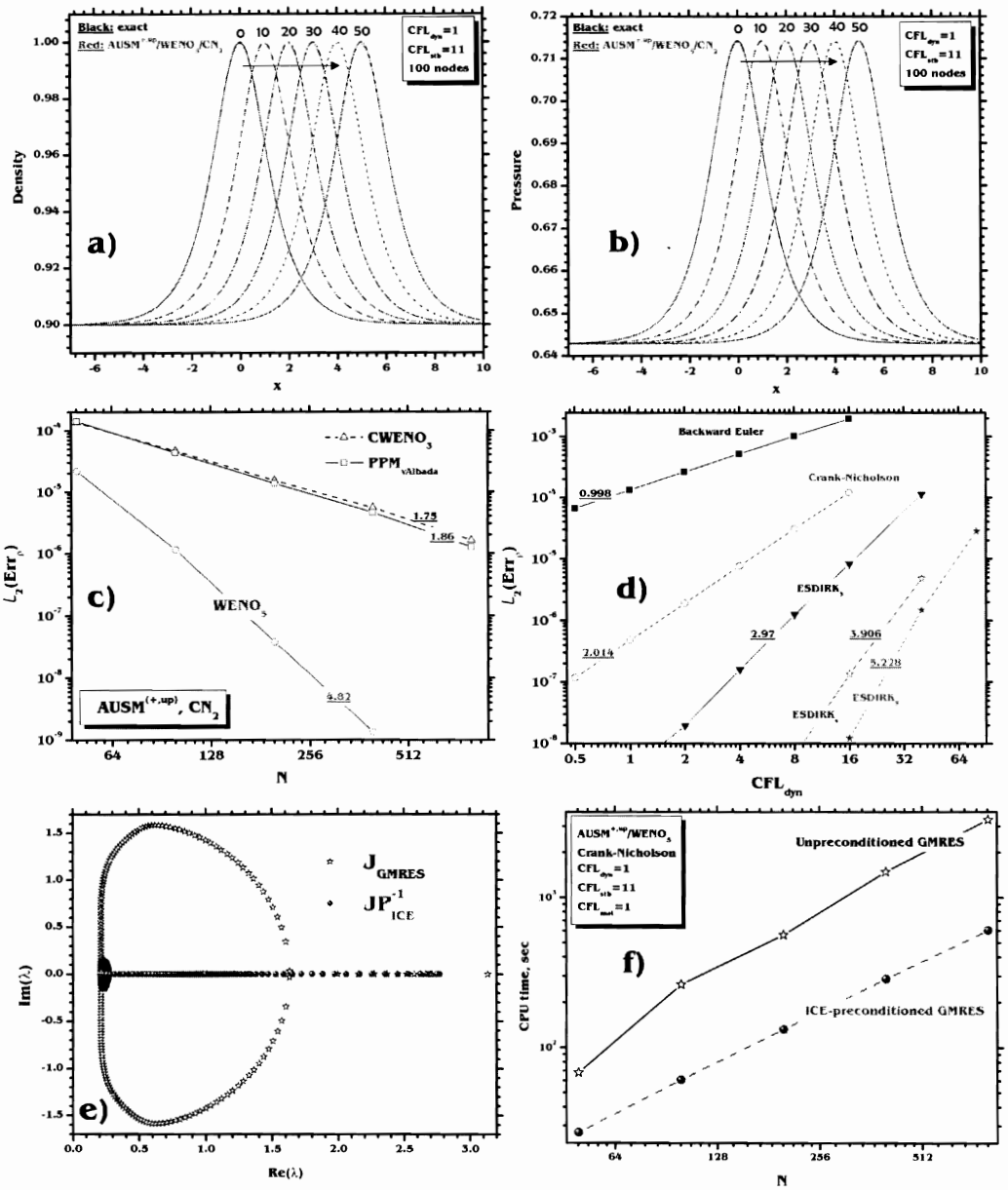

Figure 8. Illustration of the Physics-Based Preconditioning (PBP) for "Traveling Wave" manufactured solution (a,b) solved with Godunov-based, high-(up to 5^{th} in both space and time)-order discretization schemes (c,d), using Implicit Continuous-fluid Eulerian (ICE) preconditioning of compressible hydrodynamics.

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