Simulations of Multi-Phase Processes of Arc Interaction with Electrodes

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Outline

• Adaptive Mesh and Algorithm Refinement (AMAR) Framework:
  • Adaptive Cartesian Mesh
  • Kinetic & Fluid Solvers
  • Plasma Simulation Challenges
• MHD module in the AMAR Framework:
  • Convection stabilized arcs
  • Arc Deflection by Magnetic fields
  • Arc Attachment to Anode
• Cathodic Arcs as Four-Phase Systems:
  • Explosive Electron Emission in Cathodic Arcs
  • Related Phenomena: Laser ablation & Hypervelocity impact
  • Expanding Plasmas: Gas-dynamic and Plasma Phenomena
• Simulations of Arc Interactions with Electrodes:
  • Crater Formation in Cathodic Arcs
  • Taylor Cones, Free surface dynamics
• Conclusions and Future Work
Adaptive Mesh and Algorithm Refinement

- **AMAR Core:**
  - Adaptive Cartesian Mesh
  - Immersed Boundaries
  - Domain Decomposition

- **Kinetic Module:**
  - Discrete Velocity Method
  - Particle-Based Solvers (DSMC, PIC, PMC)

- **Fluid Module:**
  - Multi-species, multi-temperature
  - Chemistry (CANTERA)

- **Electromagnetics:**
  - Poisson Solver
  - DGTD Maxwell Solver

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Adaptive Cartesian Mesh

2:1 balanced grid is represented by octree. Additional constraints simplify the gradient and flux calculations:

(a) the levels of direct neighbors cannot differ by more than one;

(b) the levels of diagonal neighbors cannot differ by more than one;

Boundary Conditions

Cut-cell and IBM approaches. Cut cells are yellow, ghost cells are blue

Fully threaded tree structure for efficient traversal, access to neighbor cells, cell level and spatial coordinates

http://gfs.sourceforge.net
3D hybrid kinetic-fluid simulations of supersonic flow on a CPU-GPU NASA cluster with 58 GPU cards.

- Developed CUDA kernels for three modules in UFS: DVM Boltzmann solver, DSMC module, and LBM solver
- Double digit speedups on single GPU and good scaling for multi-GPU have been demonstrated.
- Demonstrated feasibility of porting adaptive kinetic-fluid solvers to CPU-GPU systems
- GPUs enable breakthrough Boltzmann solution with a million of kinetic cells.

Total number of adapted computational cells is 3.5M, and total number of Boltzmann cells (pink color) is ~1.2M.

Extending AMAR for Plasma Simulations

- Coupling to Electromagnetics: AMPS (Splitting vs Non-Splitting)
- Disparity of Time Scales for Electrons and Heavy Particles
- Gas mixtures & Chemical Reactions

ES-PIC-AMR: Streamer Development in Corona Discharges


Cathodic Arcs as Multi-Phase Phenomenon

- Retrograde motion of cathode spot
- Very energetic ions (energy exceeding potential drop in the cathode region)
- Multiply charged ions
- Erosion reduced with increasing ambient gas pressure
- High erosion rates in magnetically rotated arcs in air
- **Explosive electron emission** (EEE) involves metal-liquid-gas-plasma phase transition, formation of plasma jets from the EEE center (ecton), plasma jet interaction with neutral ambient gas, and multi-ecton fractal structure of the cathode spot for high current arcs.

Analogy between droplet hitting the water and vacuum arc cathode spot
MHD module in AMAR Framework

Typical 3D Arc Simulations

Computational grid colored by gas temperature (top) Isolines of electrostatic potential (bottom).

Contours of gas temperature (in K), and U velocity (in m/s)
Arc Deflection by Static Magnetic Field

Computational grid and gas temperature contours

Streamlines and gas velocity $U$ (in m/s)

Arc deflection by external DC magnetic fields,
Experiments by S. Zweben and M. Karasik,,
PPPL, 2000

Good agreement of simulation results with the experiments

3D simulation of 5 cm, 150 A arc in argon gas with external magnetic field of 2 G.
Arc Movements by AC Magnetic Field

Oscillatory motion of the arc at different frequencies and applied AC magnetic fields, Experiments by S. Zweben and M. Karasik,, PPPL, 2000

Amplitude of arc movement decreases with increasing frequency and the mode number increases, in good agreement with the experimental observations.

3D simulation of 5 cm, 150 A arc in argon gas with external AC magnetic field $B_z$ of 10 G and frequency 50 Hz. Shown on x-y slice (z-axis is perpendicular to the plane of the paper) are contours of gas temperature (in K, left column) and U velocity (in m/s; together with j-streamlines, right column) at two time instances.
Photographs of atmospheric pressure arc between a rod cathode and a planar anode for different gaps between the electrodes illustrating anode spot constriction and anode jet formation with increasing inter-electrode gap.

When the arc length reaches about 20 mm, anode spot constricts and an anode jet forms, as clearly seen at 40 mm.
Simulations of Arc Attachment to Anode

Spatial distributions of gas temperature (K) and adapted computational mesh (top) and flow velocity (bottom) for different inter-electrode gaps (10, 20 and 30 mm from left to right)

Cathode jet affects the near-anode flows for all gaps
Multi-Phase Flow Science

- Multi-Phase Flow Science deals with mixed gas-liquid-solid flows with freely moving surfaces

- Volume of Fluid and Level Set (LS) Methods:
  - Mass Conservation
  - The problem of large density ratio
  - Compressibility effects

- VOF and LS solvers with Adaptive Cartesian Mesh

- Gerris Flow Solver (GFS) includes time-dependent incompressible variable-density Navier-Stokes equations for two-fluid flow with VOF method.

Simulations of droplet impact dynamics on liquid surface with GFS
Explosive Electron Emission in Vacuum Arcs

- A distinctive feature of electric discharges in a vacuum is rapid phase transitions of the cathode material from a solid state to liquid, gaseous, and plasma states.
- The plasma state changes from a dense non-ideal to a moderately rarefied, and to a collisionless.
- The cathode material is emitted from micro-explosions (ectons) and progressively accelerated to velocities of about $10^6$ cm/s and, the particle density decreases from $10^{23}$ to $10^{10}$ cm$^{-3}$.
Ambient Gas Effects on EEE Craters

- Arc traces on cathode surfaces often contain fine structure in the form of single or overlapping craters.
- Typical diameters of such craters, as measured on clean metal surfaces, are about 10 mm. Therefore, averaged typical current densities within the spot surface are $10^{11} \text{ A/m}^2$, and power densities more than $10^{12} \text{ W/m}^2$.
- Recent experiments have confirmed similar cathode-spot mechanisms in both vacuum arcs and higher pressure arcs (up to atmospheric pressure) for currents in the range 2-50 A.
- The presence of gases may produce a surface layer, which causes a lower current per spot.

Erosion tracks of an 8 A arc on a clean W cathode in vacuum (a) and in the gas (b) (after Murzakaev, XXVIIth Int. Symp. on Discharges and Electrical Insulation in Vacuum – 2016)
Nanosecond Laser Ablation Plumes

- The pressure of ambient gas greatly influences the hydrodynamics of plume expansion.

- With air pressure increased to 100 mTorr, the plume breaks away from the target surface 50 ns after the laser onset, forming a faster moving component and a slow component near the target surface.

- At 10 Torr pressure levels, the background gas drags the plume both in the radial and in the axial directions.

Spectrally integrated and time resolved images of ns laser ablation of Cu (from Farid et al., J. Appl. Phys. 115, 033107 (2014))
Ambient Gas Effect on Laser Ablation Craters

- The common features of craters at atmosphere and in vacuum are the re-solidification of molten material in the form of whirlpools or concentric vertical ridge, turbulence, droplets, nanopores, and re-deposition of particles.
- Significant difference in the crater depth along with substantial splashing of molten material is prominent on the crater produced at atmospheric pressure than in vacuum.
- SEM images show more material removal at low pressure as compared to atmospheric pressure.
- In vacuum, the initially ejected material expands freely and the density drops rapidly.
- Ablation efficiency strongly depended on the nature and pressure of background gas.

Cu surface after laser pulses in vacuum (top) and atmospheric pressure air (bottom) (JAP 2014)
Boltzmann Kinetic Simulations of Cu Plume Expansion into Argon at 200 mTorr

Cu (top) and Ar (bottom) species densities (in $6.5 \times 10^{15}$ cm$^{-3}$), velocities (middle, in 253 m/s), and temperatures (right, in 300 K) at a time instance of 0.02 μs.

On-axis VDF of Cu atoms in log scale (iso-surfaces at level of $10^{-12}$)

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Hybrid Boltzmann-Navier-Stokes Simulations Cu Plume Expansion into Argon at 200 mTorr

Species densities, mean velocities and temperatures at 0.09 and 0.3 μs. Spatial scale is normalized to $\lambda = 10 \text{ μm}$. 

Plasma Expansion into Vacuum

Collisionless, cold ions, Boltzmann-electron model:

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \vec{u}_i) = 0, \\
m_i \frac{\partial \vec{u}_i}{\partial t} + m_i (\vec{u}_i \cdot \nabla) \vec{u}_i = -e \nabla \varphi, \\
\nabla^2 \varphi = \frac{e}{\varepsilon_0} (n_s - n_i) \\
n_s = n_0 \exp \left( \frac{e \varphi}{k_b T_s} \right)
\]

- Model strongly non-linear
- Requires dynamic grid adaptation due to fast moving plasma fronts while core plasma evolves on slow (ion) time scales
- Features highly spatially localized plasma fronts (several Debye lengths) while computational domain is from several 100’s to several 1000’s Debye lengths
- Solid objects (such as electrodes/walls) present

Currently available models:
- Uniform, structured grids (finite-difference schemes)
- Static grids (inefficient, requires user intervention to setup grid)
- Mainly Lagrangian methods (not suitable for multi-dimensional settings)
- Mainly one-dimensional
- No solid objects (such as electrodes/walls/obstacles)
Implementation on AMR Grids

A hierarchy of discretisations

- cartesian
- multigrid
- quadtree

We follow generic implementation strategies which work on different discretization hierarchies (pure Cartesian, multigrid and quad/octree) in 1D, 2D planar, 2D-axi, and full 3D settings.

Currently available schemes were adapted to 5x5 (quadtree) stencils on AMR grids for enhanced accuracy of face velocity.

Numerical model is based on staggered grid: ion density and potential are stored at cell centers (circles) and ion velocities stored at cell faces (squares).

Enhanced treatment of resolution boundaries for cell and face centered variables for static and dynamic AMR grids using restriction and prolongation operators.
Implementation on AMR Grids

- AMR + high order schemes is paramount
- Scheme adapted to dynamic AMR grids. Ion momentum equation discretized using an upwind method with explicit Euler time steps with 2\textsuperscript{nd} order accuracy finite-volume scheme on 5×5 (quadtree) & 5×5×5 (octree) stencils

- Poisson-Boltzmann equation solved by linearizing non-linear term and then converting into a Poisson–Helmholtz equation. Linear term is treated implicitly while the remaining non-linear term is treated explicitly with non-linear iterations (analog of Newton method) using a multigrid solver. Converges to specified tolerance in 2-3 linear and 5-10 non-linear iterations

- Ion continuity equation in upwind flux form, 2\textsuperscript{nd} order accuracy face reconstruction and Bell-Colella-Glaz scheme which is 2\textsuperscript{nd} order accuracy in time and space on AMR grids

\[ U^{k+1}_{\text{face}} = U^{k}_{\text{face}} - \left[ \frac{\Phi_{\text{cell}+1X} - \Phi_{\text{cell}}}{\Delta} + \max (U_{\text{face}}, 0) \frac(\vec{U} \cdot \nabla) \vec{U}

\begin{align*}
\frac{\partial U^-}{\partial X_{\text{face}}} &= \frac{3U_{\text{face}} - 4U_{\text{face}-1X} + U_{\text{face}-2X}}{2\Delta} \\
\frac{\partial U^+}{\partial X_{\text{face}}} &= \frac{-U_{\text{face}+2X} + 4U_{\text{face}+1X} - 3U_{\text{face}}}{2\Delta} \\
\frac{\partial U^-}{\partial Y_{\text{face}}} &= \frac{3U_{\text{face}} - 4U_{\text{face}-1Y} + U_{\text{face}-2Y}}{2\Delta} \\
\frac{\partial U^+}{\partial Y_{\text{face}}} &= \frac{-U_{\text{face}+2Y} + 4U_{\text{face}+1Y} - 3U_{\text{face}}}{2\Delta}
\end{align*}

1D Simulations of Plasma Expansion with AMR

- Solved on quadtree grids with vertical masking (to reduce cell count): very efficient (pure 1D treatment also possible) with grid adaptation on space charge
- Computational domain several 100’s $\lambda_D$

J. E. Allen and M. Perego, On the ion front of a plasma expanding into a vacuum, Physics of Plasmas 21, 034504 (2014);

- Very sharp ion density peaks predicted (peak widths a few $\lambda_D$)
- Good agreement with other 1D computations using both Eulerian and Lagrangian approaches. Both spatial and temporal profiles are well reproduced
- Our Eulerian code can well be used to study fast plasma expansion dynamics
The Origin of Ion Density Peaks

- Following Allen 2014, we studied the effect of a finite width over which the ion density falls to zero at \( t = 0 \).
- According to Allen 2014: the maximum electric field occurs behind the outermost ions, at the point where the electron and ion densities are equal. Positive ions at that position tend to catch up with those ahead, producing a peak in the ion density.
- Our (Eulerian) code results are in excellent agreement with these theoretical considerations and numerical results.

J. E. Allen and M. Perego, *On the ion front of a plasma expanding into a vacuum*, Physics of Plasmas 21, 034504 (2014);
Multi-Modal Ion Velocity Distributions

Initial ion-density profile plays important role in dynamics of plasma expansion
- Formation of double peaked ion-density profile is predicted for width \( l = 20 \)
- In agreement with Allen 2014 results (time and locations are different)
- This leads to formation of multi-valued (also referred to as multimodal) ion velocity distributions

J. E. Allen and M. Perego, On the ion front of a plasma expanding into a vacuum, Physics of Plasmas 21, 034504 (2014);
2D Simulations of Plasma Expansion with AMR

2D planar plasma expansion on quadtree AMR: grid adaptation on space charge

• Electric potential drop of ~8 V across the plasma front (similar to 1D)
• Narrow space charge region (ring) well resolved by AMR. Using coarse mesh in most of the regions enables an efficient computation
• Code robust and fast (both Poisson–Helmholtz solver and non-linear iterations) and handles well the levels of refinement of 10-12 required to resolve rapidly moving narrow fronts.

Conclusions:
• 2D planar extension of the collisional cold-ion model with Boltzmann electrons fully functional in Eulerian formulation
• 2D-axi implementations/testing and comparing to 3D results currently in progress
3D Simulations of Plasma Expansions from Cathode

- Extended implementations to full 3D (octree) and added capabilities to treat solid objects (such as cathodes or walls)
- AMR allows resolving well the narrow space-charge zone moving with 3-4x ion-sound speeds. The rest of computational domain (~400 $\lambda_D$) remains coarse (efficient computations and fast convergence rates)
- Expansion zone remains closely hemi-spherical above the cathode up to several 100’s $\lambda_D$
Simulations of Crater Formation on Anode Surface

3D simulation of 10 atm, 100 A arc interactions with anode: gas-liquid VOF interface and dynamically adapted grid (left), flow velocity (center, in m/s) and temperature (right, in K).

- Under these conditions, crater is formed but no droplets are emitted.

- AMR enables accurate dynamic resolution of free moving gas-liquid interface and liquid-solid boundary of the crater.
The Model of Cathode Spot

\[ \rho c_p \frac{\partial T}{\partial t} + \rho c_p \mathbf{u} \cdot \nabla T = \nabla \cdot (\lambda \nabla T) + W \]

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ \rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot \left[ -p \mathbf{I} + \mu \left( \nabla \mathbf{u} + \left( \nabla \mathbf{u} \right)^T \right) \right] + \frac{p}{l} \mathbf{n} \]

\[ W = j U_c - j \varphi_{WC} - \varepsilon \alpha T^4 - L_v \dot{m} \]

\[ \dot{m} = \frac{m_i \rho_{\text{sat}}(T)}{\sqrt{2 \pi k_B T}} \]

\[ j = j_0 \cdot \exp \left[ -\left( \frac{r}{a} \right)^2 \right] \cdot \theta(t - \tau) \]

\[ \frac{p}{l} \mathbf{n} = \left( \frac{p_{\text{sat}}(T)}{l} + \sigma \kappa \right) \delta_a \mathbf{n} \]

Predicted temperature and flow velocity

Plasma pressure was calculated as the saturated vapor pressure for a given surface temperature.

Arc current 3 A; spot radius 5 µm; spot lifetime 10 ns
An Example of Crater Dynamics

$t = 9$ ns
Black line shows where $T > T_{\text{melt}}$

$t = 28$ ns

$t = 60$ ns
Splashing vs Spreading

Boundaries between the spreading and the splashing regimes; from Gashkov and Zubarev, J. Phys.: Conf. Series 946, 012131 (2018)

Weber and Reynolds numbers:

\[ \text{We} = \rho U^2 D / \sigma \]
\[ \text{Re} = UD / \nu \]

Fig. A obtained by increasing surface tension 10 times in order to increase \( \text{We} \) and obtain spreading regime.
Fig. B obtained by decreasing viscosity 10 times in order to obtain splashing regime: the liquid pool ejects many bubbles.
Formation of Taylor Cone on Cathode Surface

3D simulations of micro-protrusion formation on cathode surface: contact VOF surfaces at 3 time instances, dynamically adapted grids, and contours of vertical electric field (in V/m). Surface tension coefficient $\sigma_s = 0.4$ N/m.

Our simulations have shown that using adapted computational grid helps adequately resolving the dynamics of free liquid surface, Taylor cone formation, and liquid droplet ejection.

Surface tension force at the gas-liquid interface is important for accurate predictions of the protrusion formation and associated EEE phenomena.
Conclusions & Future Work

- We have applied the AMAR methodology for simulations of plasma expansions.
- The Volume of Fluid (VoF) model with AMR has been applied to modeling gas-liquid-solid flows with free surfaces.
- Experiments are under way to study single ecton generation on liquid cathodes for different gas pressures.
- Integration of plasma and VoF capabilities is under way for simulations of EEE and related phenomena.

Shadow photographs showing the (a) growth and (b) decay of a protrusion on the liquid metal cathode with diameter 4 mm

Proskurovsky, Explosive Electron Emission From Liquid-Metal Cathodes, IEEE TPS 2009
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